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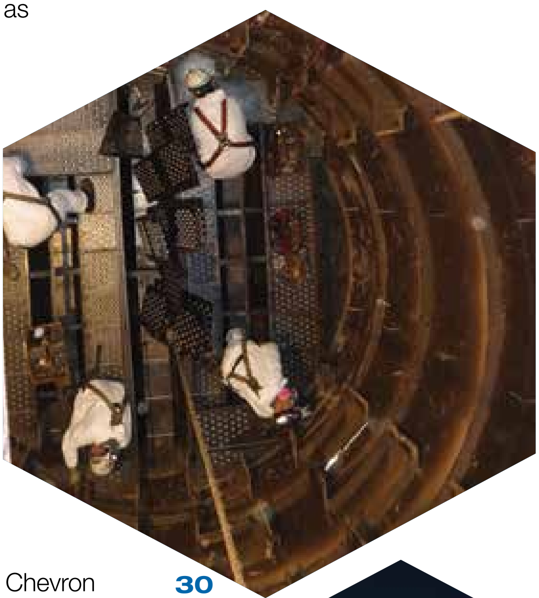
Cover Story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Editor's Page

Engineering energy

The chemical process industries (CPI) influence much of what affects our daily lives in areas as diverse as agriculture, pharmaceuticals, food products, basic chemicals and more. One field where many engineers are focusing their efforts is energy. Efforts toward widening energy resources beyond petroleum and shale gas reserves have R&D experts looking at alternate renewable resources and the technologies needed for a shifting energy landscape.

Trends

A strong trend in the energy sector is the decentralizing of energy generation, which includes an upswing in renewable energy sourcing. Recently, the European Parliament (www.europarl.europa.eu) endorsed proposals for an aggressive renewable energy target of 35% of E.U. energy consumption to be from renewable sources by 2030. In the U.S., states are setting their own energy goals. Hawaii touts the most aggressive goals in the nation, with a target of 100% "clean" energy by 2045. And at least 29 states have renewable energy targets, as reported by the National Conference of State Legislatures (www.ncsl.org) on its website. In addition to renewable energy mandates, several states also have energy storage programs and targets. The New York State Energy Research and Development Authority (NYSERDA; www.nyserda.ny.gov), for example, is making $6.3 million available for energy storage technology and product development to accelerate energy storage deployment.

Technology challenges

Renewable energy initiatives have been a driver for technological advances in the field, and chemists and engineers are well-equipped to address many of the technical challenges. Numerous CPI companies are invested in various types of renewable energy work. As just one example, last year Borealis AG (www.borealisgroup.com) and Borouge formed a partnership for innovations in solar energy through their newly created Quentys brand.

And, one of the biggest challenges in the growing renewable energy field is the need to control the variability in the energy availability through energy storage. Much work on energy storage options is being carried out by the CPI and universities, resulting in frequent announcements of new developments. See, for example, "Progress towards an aluminum-graphene battery" on p. 7 of this issue, and "A step closer for graphene-coated anodes" on p. 6 of our January issue.

New developments in the CPI

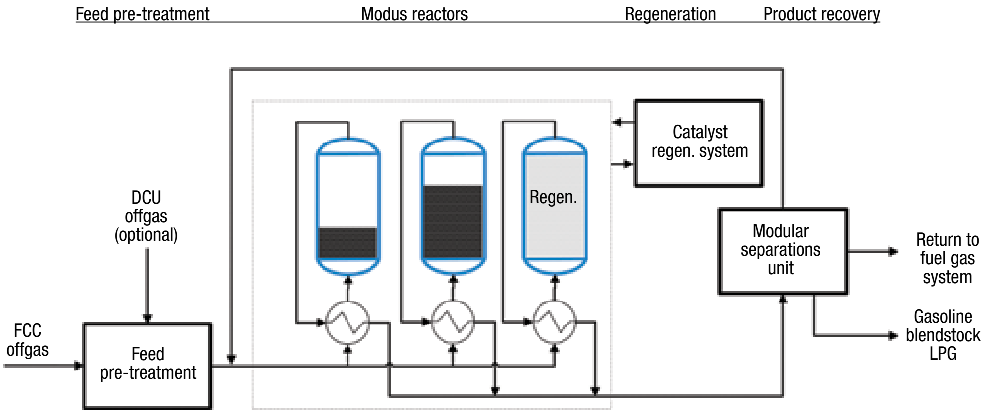
In addition to the work on energy generation and storage, CPI companies are also investigating alternative energy sources and ways to increase energy efficiency within their own processes. One area gaining attention is to mimic photosynthesis in reactors. As an example, see "Making ethylene by artificial photosynthesis" on p. 7 of our January issue.

Evonik (www.evonik.com) and Siemens (www.siemens.com) recently announced the launch of a joint research project to use power from renewable sources and bacteria to convert CO_2 into specialty chemicals. The project, called Rheticus, will involve electrolysis and fermentation processes.* Keep tuned to the pages of *Chemical Engineering* for more on the many ways in which chemists and engineers are contributing to the changing energy landscape. ■

Dorothy Lozowski, Editorial Director

*For a short video on Rheticus, see www.youtube.com/watch?v=eCt0bgZn9Ws&feature=youtu.be

New process converts refinery offgas into gasoline



A process technology that upgrades offgas from petroleum refineries has been commercialized by Siluria Technologies Inc. (San Francisco, Calif.; www.siluria.com) and Wood (Aberdeen, Scotland; www.woodplc.com). According to Siluria, the new Modus technology's ability to chemically convert refinery offgases into high-quality gasoline products is an industry first. Other technologies to treat offgases involve more complex purification and cryogenic separation steps that result in products that can present logistical or economical challenges to the petroleum refinery.

The Modus process (diagram) converts light olefins contained in the offgas from refinery operations, such as a fluid catalytic cracker (FCC) or a delayed coker unit (DCU), into a gasoline blendstock. In the Modus process, offgas is pre-treated using compression and simple guard beds. It is then fed to a reaction system, which oligomerizes the offgas' olefin content into longer hydrocarbon chains. This reactor system, which can include three to five reactors, depending on the desired capacity, consists of parallel adiabatic fixed-bed reactors that contain a proprietary catalyst. The reactors run continuously in a swing or cyclic mode, meaning that one reactor can be kept offline to regenerate the catalyst while the others operate in swing mode. Since the Modus catalyst was specially designed for compatibility with offgas streams, the technology is simple to integrate into most refinery settings. The Modus process can also result in reduced overall site emissions, since combustion of unsaturated offgas components is no longer necessary.

In tests at Siluria's pilot facilities, the process has been shown to produce liquid product output of several gallons per day. Siluria and Wood used this pilot system to develop the commercialized modular engineering design package. The partners are now in discussion with multiple refining companies and plan to commence pre-FEED (front-end engineering design) studies in the first half of 2018.

Edited by:
Gerald Ondrey

RE-FREE MAGNETS

Tetrataenite ($L1_0$-FeNi) is a promising alternative to rare-earth- (RE) based magnets due to its favorable magnetic properties, such as a high uniaxial magnetic anisotropy and saturation magnetic-flux density. Compared to other non-RE alternatives, such as Nd-Fe-B and Sm-Fe-N, which have a low thermal resistance, $L1_0$-FeNi has a Curie point of ≥550°C, which is higher than conventional magnets. However, $L1_0$-FeNi has only been found naturally in trace amounts in meteorites, so efforts to make the highly ordered alloy have been underway. Now, a Japanese collaboration, led by Denso Corp. (Aichi; www.denso.com), with support of the New Energy and Industrial Technology Development Organization (NEDO; Kawasaki; www.nedo.go.jp), has succeeded in synthesizing high-purity $L1_0$-FeNi for the first time, as reported in a recent issue of *Scientific Reports*.

The researchers developed a technique for ordering atoms in an alloy called nitrogen insertion and topotactic extraction (NITE). In this method, the ordered arrangement of Fe and Ni, with nitriding as the trigger, is combined with

(Continues on p. 8)

Startup for a demonstration plant to process three metals

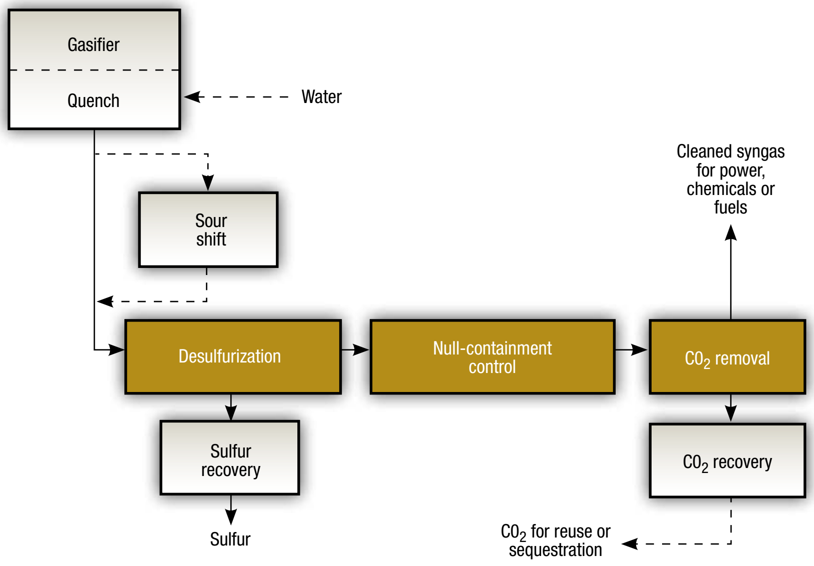
Australian Mines (Perth; https//:australianmines.com.au) has started operating a demonstration cobalt-nickel-scandium processing plant that will process ore from the company's Sconi and Flemington projects into commercial-grade samples.

The company's flagship Sconi project, located in the mining center of Greenvale in Queensland, is based on an estimated average production of 3,000 metric tons per year (m.t./yr) of cobalt sulfate, 24,420 m.t./yr of nickel sulfate and 77 m.t./yr of scandium oxide for the first 20 years. The Sconi project can produce the raw materials required in a Tesla Model S battery pack cathode, which is comprised of 80% Ni and 15% Co.

The Flemington project, located 370 km west of Sydney in New South Wales, is a direct continuation of the Sunrise Project under development by Clean TeQ Holdings Ltd., with the two projects separated only by a tenement boundary. The Flemington project has an estimated 89 million m.t. of ore at an expected average feed grade of 0.11% Co, 0.80% Ni and about 0.011% Sc.

The demonstration plant uses a conventional pressure acid-leach front-end to dissolve the metals into solution. It includes a solid-liquid separation and standard solvent extraction and sulfate crystallization back-end to separate out the Co, Ni and Sc to produce final products. With a throughput capacity of 2,200 kg/d of ore, the plant can deliver a weekly output of 67 kg of cobalt sulfate ($CoSO_4{\cdot}7H_2O$), 500 kg of nickel sulfate ($NiSO_4{\cdot}6H_2O$) and 8 kg of scandium oxide (Sc_2O_3).

Lower-cost sulfur-removal process for syngas goes commercial



An adsorbent-based, sulfur-removal process for synthesis gas (syngas) that lowers capital and operating costs compared to alternative methods of removing sulfur has completed pre-commercial testing and has achieved commercial status. The Warm-gas Desulfurization Process (WDP; diagram) has been under development by Research Triangle Institute (RTI; Research Triangle Park, N.C.; www.rti.org) for over 10 years, and is now commercially available through RTI's partner Casale S.A. (Lugano, Switzerland; www.casale.ch). A proprietary solid-sorbent material critical to the process is now being manufactured by another RTI partner, Clariant (Muttenz, Switzerland; www.clariant.com).

RTI says that the WDP technology consistently reduced inlet total sulfur by 99.8–99.9% in raw syngas with sulfur concentrations as high as 14,000 parts per million (ppm). Further, integration of WDP with CO_2-capture systems can reduce sulfur to parts-per-billion levels, according to RTI, which renders the syngas suitable for chemicals-, fertilizer- and fuel-manufacturing processes. "Removing sulfur at warm process temperatures contributes to increased efficiencies and lower operating and capital expenditure," RTI says.

To remove sulfur from syngas, WDP uses a dual transport reactor, where the first reactor adsorbs sulfur compounds from the raw syngas while the second reactor regenerates the sorbent material, RTI explains. RTI points out that one of the unique factors of the process is its ability to operate at pressures up to 80 bars, which matches many commercial gasifier systems. "Keeping process conditions constant contributes to increased efficiencies and lower operating and capital expenditure," RTI says.

WDP was first piloted at a coal gasification unit at Eastman Chemical Co. (Kingsport, Tenn.; www.eastman.com) and then scaled up at a pre-commercial testing unit in Florida that removed sulfur from coal-derived syngas at an integrated gasification combined cycle (IGCC) power plant (*Chem. Eng.*, August 2010, p. 10).

Since the initial pilot plant, RTI and Clariant have made improvements to the novel sorbent material, including, among other things, an improved manufacturing process that effectively disperses the active metals, allowing high sulfur capacity and fast reaction rates.

Biomass fractionation and conversion technology to be scaled up

Plans are underway for a demonstration-scale facility in France that will convert non-food lignocellulosic biomass into raw materials for bio-based chemicals and animal feed products, such as feed for fish farming. The process, developed by Arbiom (Research Triangle Park, N.C.; www.arbiom), is currently operated at pilot scale at a facility in Norton, Va. The Arbiom process efficiently separates agricultural and forestry waste biomass into its constituent components: C5 sugars, C6 sugars and lignin. The products will be used for making bio-based chemicals, feed and other products.

"It's challenging to efficiently convert cellulose, which is primarily in a crystalline form, into the C6 sugar glucose using today's enzymes," explains Arbiom chief operating officer Marc Chevrel. "So we are upscaling a proprietary phosphoric acid pretreatment process for the biomass that generates amorphous cellulose, which is more highly reactive and more easily hydrolyzed by industrial enzymes into glucose."

The pretreatment step occurs under mild process conditions and has been designed to simplify the development of Arbiom's optimized enzyme cocktails. This lowers operational costs. Along with a partner, the company has also developed a phosphoric acid recycling system to re-use the acid.

Beginning with a material such as sawdust, Arbiom's biomass fractionation process first separates hemi-cellulose, which is converted into the C5 sugar xylose. Then cellulose is separated to be enzymatically converted to glucose. The reactions are carried out in specially adapted reactors. While the pilot plant has used batch reactors, the demonstration facility in development will move toward continuous production, Chevrel says.

Construction of the 5,000-ton/yr demonstration-scale plant is being supported by grants from the European Union Bio-Based Industries Joint Undertaking (BBI-JU) and from the French government. The plant will be co-located with a pulp-and-paper production facility in eastern France to take advantage of material transport logistics. Arbiom is working with partners to use the sugars generated in its process for biologically derived products, and is investigating several applications for the lignin from the fractionation process.

Progress towards an aluminum-graphene battery

Compared to conventional lithium-ion batteries, aluminum-ion batteries (AIBs) offer significant advantages, such as non-flammability, and a high capacity of the metallic Al anode. However, due to inadequate cathodic performance, especially capacity, high-rate capability and cycle life, AIBs cannot compete with Li-ion batteries and supercapacitors. The energy density of AIBs (40–60 Wh/kg) is much lower than that of commercialized Li-ion batteries (150–250 Wh/kg), and AIBs' power density (3–30 kW/kg) and cycle life (200–25,000 cycles) are lower than those of advanced supercapacitors (30–100 kW/kg and 10,000–100,000 cycles).

The following four basic requirements should be fulfilled simultaneously for a desired carbon-based cathode: 1) Highly crystallized defect-free graphene lattice as an active anion intercalation site affording suitable energy storage capacities; 2) Continuous electron-conducting matrix for large current transport and internal polarization mitigation; 3) High mechanical strength and Young's modulus to prevent material collapsing during repeated anion intercalation and de-intercalation; and 4) Interconnected channels facilitating high electrolyte permeability, ion diffusion and fast redox reactions between electrolyte and active material.

To find a new design to upgrade the cathode performance of AIBs, a team from Zhejiang University (Hangzhou, China; www.zju.edu.cn), led by professor Gao Chao, has proposed a "tri-high tri-continuous (3H3C) design" to achieve the ideal graphene film (GF-HC) with good electrochemical performance.

Ordered assembling of graphene liquid crystal led to a highly oriented structure, satisfying requirement Number 3 mentioned above. High-temperature annealing and concomitant "gas pressure" contributed to the good quality and yet high-channeling graphene structure that met Requirements 1, 2 and 4.

Due to its targeted 3H3C design, the resulting aluminum-graphene battery achieved ultralong cycle life (91.7% retention after 250,000 cycles), high-rate capability (111 mAh/g at 400 A/g based on the cathode), wide operating temperature range (from –40 to 120°C), flexibility and non-flammability.

However, Gao says, the AIB cannot yet compete with commonly used Li-ion batteries in terms of energy density, or the amount of power that can be stored in the battery. It is still too costly to make such a battery, Chao says. He adds that commercial production of the battery can only become possible when a less-expensive electrolyte is found.

The results of the study were published in a recent issue of *Science Advances*.

topotactic denitriding for extracting nitrogen atoms from Fe-Ni nitrides without damaging the crystal structure. The proposed method is significantly different from the conventional thermally activated process in that the ordered alloys can be derived directly by denitriding.

The proposed method not only significantly accelerates the development of magnets using $L1_0$-FeNi, but also offers a new synthesis route to obtain ordered alloys in non-equilibrium states. Such alloys can have improved mechanical (toughness) and catalytic properties.

DNA CAGES AS MOLDS

Researchers from McGill University (Montreal, Que., Canada; www.mcgill.ca) have chemically imprinted polymer particles with DNA strands — a technique that could lead to new materials for applications ranging from biomedicine to the promising field of "soft robotics" (robotics made with soft, flexible structures that can change shape in response to external stimuli). The method, described in a recent issue of *Nature Chemistry*, "introduces a programmable level of organization that is currently difficult to attain in polymer chemistry," says McGill chemistry professor Hanadi Sleiman, senior author of the study. "Chemically copying the information contained in DNA nanostructures offers a powerful solution to the problem of size, shape and directional control for polymeric materials."

Although polymers are widely used, most self-assembled polymer structures have been limited to symmetrical forms, such as spherical or cylindrical shapes. Recently, however, scientists have focused on creating non-symmetrical polymer structures — for example "Janus" particles with two different "faces" — and they are starting to discover new applications for these materials.

Together with colleagues at the University of Vermont and Texas A&M University at Qatar, the McGill researchers developed a method to imprint a polymer ball with DNA strands arranged in pre-designed orientations. The cages can then be undone, leaving behind DNA-imprinted polymer particles capable of self-assembling — much like DNA, itself — in pre-designed patterns. Because the DNA cages are used as a "mold" to build the polymer particle, the particle size and number of molecular units in the polymer can be precisely controlled, says Sleiman.

BIO-BASED COSMETICS POLYMER

Clariant (Muttenz, Switzerland; www.clariant) and Global Bioenergies (Evry, France; www.global-bioenergies.com) have developed a polymer for cosmetic creams and lotions that is derived from renewable isobutene. Developed with Global Bioenergies' sugar-based isobutene, Clariant's new ingrediant is a rheological modifier that influences formulation viscosity, and achieves specific sensorial and texturizing properties for creams and lotions. It contains more than 50% renewable carbon.

The isobutene feedstock is currently being produced on a small scale at Global Bioenergies' demonstration plant in Leuna, Germany. The two companies are working on upscaling production with larger volumes. ❑

Catalytic advances enable conversion of methane without coking . . . .

The large supply of unconventional natural gas from shale deposits in the U.S. has increased attention on utilizing small alkanes to synthesize higher-value chemicals and fuels, while avoiding thermal steam-cracking, which is energy-intensive. Attempts to catalytically convert methane, ethane and propane to industrially relevant chemicals, such as methanol, ethylene, propylene and others, require activation of the relatively inert carbon-hydrogen bond in alkanes. A team of researchers from Tufts University (Medford, Mass.; www.tufts.edu) has advanced the effort toward catalyst-aided reaction of small alkanes in a series of recent papers.

In one study, published in *Nature Chemistry*, the team investigated a catalyst system designed to avoid the problem of deactivation by coke buildup, which has plagued many platinum- and nickel-based catalyst systems in this area. Both can activate C–H bonds, but tend to dehydrogenate alkanes completely, leading to coking. The Tufts researchers investigated a single-atom alloy (SAA) composed of 1% individual, isolated platinum atoms in a copper surface. Copper is resistant to coking, but does not have the ability to activate C–H bond breakage. So the introduction of dispersed, individual atoms of platinum in the copper matrix facilitates catalytic activity without the coke formation.

The development of SAA catalysts was enabled by scanning tunneling microscopy imaging of Charlie Sykes, a Tufts chemistry professor who led the study. "Using this surface-imaging technique, we could visualize model surfaces with single-atom resolution and relate these structures to the chemistry that we observed," Sykes remarks.

"By distributing Pt atoms in a copper surface, we lose some activity, but we gain significantly in our ability to use Pt in the only form that can give us the dehydrogenation products we want at low temperatures and without deactivation," says Maria Flytzani-Stephanopoulos, a Tufts professor of chemical engineering who co-led the research. The experimental work at Tufts was aided by Michail Stamatakis at University College London, who performed quantum calculations.

. . . and direct conversion of methane to methanol and acetic acid

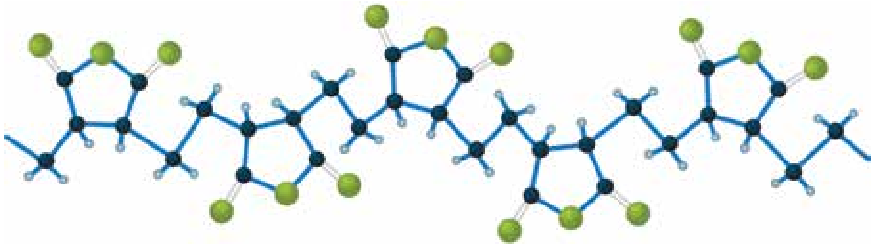
In another recent paper, published in *Nature*, the Flytzani-Stephanopoulos group (see above) identified a new method of converting methane directly into methanol or acetic acid under mild conditions using oxygen, carbon monoxide and a heterogeneous rhodium catalyst. This is said to be the first such demonstration in the scientific literature.

The researchers synthesized single-atom rhodium species anchored on the internal walls of zeolites or on the surface of titanium oxide (TiO_2) supports. These materials catalyze the direct oxidation of methane with oxygen and carbon monoxide in aqueous solutions. A key aspect of the catalyst synthesis was atomically dispersing the rhodium species, the researchers say. This was achieved by "a special heat-treatment protocol on the zeolite support and by anchoring the rhodium precursor species on reduced titania assisted by ultraviolet irradiation," the group says.

The reactions were carried out under mild pressures (20–30 bars) and temperatures (<150°C). The researchers found that carbon monoxide is essential to the gas mixture in order to produce methanol. Also, by carefully controlling the reaction conditions, particularly the acidity of the support, the team could produce either methanol or acetic acid.

With further study, the process could be developed into a more energy-efficient and environmentally friendly way of producing methanol and acetic acid than current indirect processes, according to Flytzani-Stephanopoulos.

Recycled materials improve the nylon product chain



Although recycled polymers can provide sustainable, low-cost feedstock, their use is challenging in applications that require high-performance characteristics. Vertellus LLC (Indianapolis, Ind.; www.vertellus.com) has developed additives to improve processors' ability to incorporate recycled nylons and recycled polyesters into virgin nylon. One such additive, ZeMac, has been used in films and coatings as a coupling agent, but Vertellus has also validated its use as a plastic additive to improve the mechanical properties of recycled nylon streams. Typically, engineering thermoplastics and other injection-molding applications cannot incorporate recycled nylon due to the inconsistent properties of the stream, explains Vertellus' marketing manager Prasad Taranekar. With ZeMac, processors can create a mixed stream of virgin and recycled nylon exhibiting uniform consistency and controlled viscosity, along with improvements in other critical properties.

ZeMac's chemical structure (diagram) sets it apart from other additives used for nylon processing thanks to a specialized polymerization process that results in a very high concentration (78 wt.%) of maleic anhydride alternating with ethylene. Maleic anhydride enables faster reactions in compounding operations, as well as much lower additive dosing rates. According to Taranekar, most comparable additives have less than 5 wt.% maleic anhydride.

Vertellus is also developing another additive technology that targets incorporation of recycled polyester into virgin nylon streams, as well as upgrading recycled polyester itself. Nylon and polyester do not mix well, says Taranekar, so the additive must facilitate micro-level phase mixing, as well as imparting the appropriate mechanical properties. "Recycled polyesters' viscosity is not suitable for injection molding, so what we want to do is boost the intrinsic viscosity while also enhancing the mechanical properties and hydrolytic stabilities," he adds. Vertellus is currently testing the technology at customer sites and is seeking strategic partners for a commercial rollout. "As far as I know, there is no other product on the marketplace aimed at combining recycled polyester and virgin nylon," he comments. ■

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Plant Watch

Asahi Kasei to increase global production capacity for LIB separators

January 11, 2018 — Asahi Kasei Corp. (Tokyo, Japan; www.asahi-kasei.co.jp) will increase production capacity for lithium-ion battery (LIB) separators at its plants in North Carolina and Shiga, Japan. In North Carolina, the facility's capacity will expand to 150 million m^2/yr, with startup scheduled in the second half of fiscal 2018. In Shiga, the facility will be expanded to 90 million m^2/yr, with startup scheduled in the first half of fiscal 2020.

Sinopec to use Eni's slurry technology for new refinery unit

January 9, 2018 — Sinopec (Beijing, China; www.sinopecgroup.com) will construct a new plant based on Eni S.p.A.'s (Rome, Italy; www.eni.com) Slurry Technology with a design capacity of 46,000 barrels per day (bbl/d) of heavy petroleum-refining residue. The plant is due to be completed by 2020. The new plant will be built at Sinopec's petroleum refinery in Maoming, in Guandong province.

Enterprise Products to expand butane isomerization capacity in Mont Belvieu

January 9, 2018 — Enterprise Products Partners L.P. (Houston; www.enterpriseproducts.com) plans to expand its butane isomerization facility at its complex in Mont Belvieu, Tex. Enterprise is currently evaluating two options to expand its butane isomerization facilities that would add up to 30,000 bbl/d of incremental capacity.

Evonik to build new PMMA compounding line at Arkansas site

January 8, 2018 — Evonik Industries AG (Essen, Germany; www.evonik.com) will construct an additional line for compounding polymethyl methacrylate (PMMA) at its site in Osceola, Ark. The expansion will nearly double the production capacity of the Methacrylates business line for the specialty molding compounds produced there. Completion and startup of the new compounding line is scheduled for the first quarter of 2019.

Celanese announces startup of polyacetal plant in Saudi Arabia

January 3, 2018 —Celanese Corp. (Dallas, Tex.; www.celanese.com) says that the Ibn Sina joint venture successfully started up its polyacetal manufacturing facility in Jubail Industrial City, Saudi Arabia, which has a production capacity of 50,000 metric tons per year (m.t./yr). Ibn Sina is a joint venture between Saudi Basic Industries Corp. (Sabic; Riyadh, Saudi Arabia; www.sabic.com) and CTE, a company jointly owned by subsidiaries of Celanese and Duke Energy.

Chevron Phillips' Cedar Bayou ethane cracker reaches mechanical completion

December 28, 2017 — Chevron Phillips Chemical Co. LP (The Woodlands, Tex.; www.cpchem.com) successfully achieved mechanical completion of its ethane cracker at Cedar Bayou in Baytown, Tex. The unit is now undergoing commissioning activities, system checks and final certifications. Once operational, the unit is expected to produce 1.5 million m.t./year of product.

Stamicarbon wins contracts for a new, ultra-low-energy urea plant in China

December 23, 2017 — Stamicarbon B.V. (Sittard, the Netherlands; www.stamicarbon.com) and Jiujiang Xinlianxin Fertilizer Co. (XLX) have signed contracts for technology licensing and delivery of proprietary equipment for a new ultra-low-energy urea plant to be built in Jiujiang, Jiangxi, China. Plant startup is planned for the end of 2020.

Sibur to expand terephthalic acid production capacity

December 20, 2017 — Sibur (Moscow; www.sibur.com) has launched an expansion project to increase terephthalic acid production capacity at its Polief Blagoveshchensk site to 350,000 m.t./yr. The upgrade project impacts 11 existing production units. The project is scheduled for completion in 2019.

AkzoNobel plans to increase production of high-purity salt at Delfzijl site

December 20, 2017 — AkzoNobel's (Amsterdam, the Netherlands; www.akzonobel.com) Specialty Chemicals business plans to expand the production of high-purity vacuum salt at its Delfzijl site in the Netherlands. The project would increase output at the facility by around 25%. AkzoNobel aims to complete the project within three years.

BASF and Sinopec to expand production capacity for neopentylglycol in Nanjing

December 20, 2017 — BASF SE (Ludwigshafen, Germany; www.basf.com) and Sinopec will expand the production of neopentylglycol at a joint site in Nanjing, China. The expansion will double the Nanjing site's capacity from 40,000 m.t./yr to 80,000 m.t./yr. The expanded capacity will come onstream in 2020.

Mergers & Acquisitions

Air Products to acquire gasification business and patent portfolio from Shell

January 10, 2018 — Air Products (Lehigh Valley, Pa.; www.airproducts.com) will acquire Royal Dutch Shell p.l.c.'s (The Hague, the Netherlands; www.shell.com) Coal Gasification Technology business, as well as Shell's patent portfolio

for liquids gasification. In addition, the two companies also formed a strategic alliance in liquids gasification.

PolyOne acquires Spain-based masterbatch provider IQAP

January 4, 2018 — PolyOne Corp. (Cleveland, Ohio; www.polyone.com) acquired IQAP Masterbatch Group S.L., a privately owned provider of specialty colorants and additives based near Barcelona, Spain with customers throughout Europe. IQAP has two production facilities and a technology laboratory located in Spain, plus additional manufacturing capability in the Czech Republic.

Synthomer divests production site in Leuna, Germany

January 2, 2018 — Synthomer p.l.c. (London, U.K.; www.synthomer.com) sold its site in Leuna, Germany to Alberdingk Boley GmbH for an undisclosed price. The Leuna site was acquired as part of the Hexion PAC acquisition in 2016. This sale will conclude the integration of Hexion PAC into the Synthomer Group.

Umicore to acquire metathesis catalysts business from Materia

December 28, 2017 — Umicore N.V. (Brussels, Belgium; www.umicore.com) agreed to acquire Materia's metathesis catalyst business portfolio for a price of $27 million. Through this acquisition, Umicore will broaden its range of catalyst technologies and expand its homogeneous catalysts offering. The transaction is subject to closing conditions and is expected to be finalized in the first quarter of 2018.

CB&I to merge with upstream service provider McDermott International

December 20, 2017 — McDermott International, Inc. (Houston; www.mcdermott.com) and CB&I (The Woodlands, Tex.; www.cbi.com) have agreed to combine, creating a vertically integrated onshore-offshore company. Upon completion of the transaction, McDermott shareholders will own approximately 53% of the combined company and CB&I shareholders will own approximately 47%. The estimated enterprise value of the transaction is approximately $6 billion.

Celanese to acquire thermoplastics compounder Omni Plastics

December 20, 2017 — Celanese agreed to acquire Omni Plastics and its subsidiaries, including the distributor Resinal de Mexico. Omni Plastics is headquartered and has a compounding facility in Evansville, Ind., with additional offices in Mexico City. Omni Plastics specializes in custom compounding of various engineered thermoplastics.

W.R. Grace to acquire Albemarle's Polyolefin Catalysts business

December 15, 2017 — W.R. Grace & Co. (Columbia, Md.; www.grace.com) will acquire the Polyolefin Catalysts business of Albemarle Corp. (Charlotte, N.C.; www.albemarle.com) for $416 million. The acquired business provides proprietary and custom-manufactured catalysts, as well as metallocenes and activators. The acquisition also includes a comprehensive series of highly optimized Ziegler-Natta catalysts for polyethylene production. ■

Mary Page Bailey

Placing Analytics in the Hands of Engineers

The field of data analytics is evolving quickly, and an increasing number of tools are being designed with chemical engineers in mind

IN BRIEF

DESIGNING TOOLS FOR END USERS

PREDICTING THE FUTURE WITH BIG DATA

FIGURE 1. Advances in data science and analytics are rising to the unique challenges of CPI operations and are beginning to capture the value of the rapidly evolving industrial IoT

Big data, smart devices, Internet of Things (IoT) — these are terms heard more and more frequently in the chemical process industries (CPI). But as connectivity proliferates, questions arise about how CPI facilities can best make use of the wealth of data they are collecting (Figure 1). "Data analytics are here to stay — those who don't use it will lose out to competitors who do," says Petri Vasara, vice president of management consulting at Pöyry plc (Helsinki, Finland; www.poyry.com). These benefits reach beyond process improvements into more esoteric areas, such as safety and sustainability. Vasara lists minimizing raw materials consumption and reducing emissions as two specific environmental benefits realized by data analytics. "Modern process-control equipment provides significant amounts of data that can be used for proactive disturbance elimination and process stabilization, promoting not only safety, but higher efficiency and sustainability," explains Tom Lind, vice president of technology and new solutions at Pöyry. Introducing these principles into CPI sites will require continued dedication and diligence — integrating new elements piece by piece, and improving upon existing solutions, mentions Vasara. "It's an evolution rather than a revolution," he emphasizes.

Designing tools for end users

Although data availability and analysis technologies have made massive strides in recent years, these platforms are limited if end users cannot easily apply them. TrendMiner (Hasselt, Belgium; www.trendminer.com) provides an advanced analytics platform that engineers can use to analyze, monitor and predict massive time-series data. "We are aware that the engineers we work with are not data scientists, but chemical engineers. They have a different background and different questions arise for them," says Thomas Dhollander, chief technology officer and co-founder of TrendMiner. "We identified a number of day-to-day questions that process experts are confronted with, and we found ways to answer them," he explains.

Giving engineers the ability to interpret their own data in ways that make sense to them reduces the bottleneck of bringing in data scientists to provide insight. For instance, an engineer looking to diagnose a fouling problem could search for similar instances in the history of a unit and develop and validate a hypothesis for future operational anomalies. The system can recommend certain parameters to suggest root causes and compare events, and it can even reveal early indicators for adverse asset behavior. "You can basically create communication channels across the plant about possible early indicators so operators can intervene before abnormal situations occur," says Dhollander. Another benefit, explains Edwin van Dijk, TrendMiner's vice president of marketing, is ensuring that assets

operate in an optimal operating zone that is less stressful so that they can run longer.

The company recently worked with Covestro AG (Leverkusen, Germany; www.covestro.com) to initiate an energy-savings project at Covestro's site in Antwerp, Belgium. Energy consumption was logged and compared with historical values, looking for unexpected spikes in consumption. This led to an examination of steam use, and the team reconfigured a control scheme to prevent reactor temperature fluctuations caused by spontaneous heating and cooling. These types of comparative analytics are also useful in other improvement areas, such as the reduction of cycle times in batch processes, mentions Van Dijk.

Dhollander believes that the growing awareness of data's value will be transformative to the CPI. "Data science evolution is happening in different areas in parallel, and this will lead to a better understanding of processes and make new products or business models possible," he adds. The self-service approach lends itself to faster adoption, he explains, because there is no steep learning curve for process experts to begin using the tools. The next generation of data analytics may become even more accessible, as TrendMiner developers are looking to other markets for inspiration, including the creation of a "recommendation engine" modeled after e-commerce websites. "When working with measurement data, you will be presented with relevant suggestions of early indicators that potentially relate to an anomaly you're studying," he says.

Michael Risse, vice president of Seeq (Seattle, Wash.; www.seeq.com) further underlines the importance of direct interaction between engineers and their process data without requiring assistance from data scientists, and the ability to share those data across organizations and enterprises. "This makes it easier to collaborate, in realtime if required, across teams and sites by providing a productive and organization-friendly approach," says Risse. Seeq provides a network of connectors to organize and analyze process data housed in historians and other data sources, without moving or copying the data. This enables engineers to query and interact with the data without modifying the source itself. Seeq has seen success using its data cleansing and capsule technologies to eliminate noise from sensors, allowing users to quickly identify critical operating conditions contributing to adverse situations, such as fouling. A focus on root causes eliminates the false positives that are sometimes seen in other analytical approaches, making it easier to determine optimal conditions and avoid outages, explains Risse.

Looking forward, Risse believes that to truly embrace modern data-analytics capabilities, companies need to break the mold. "The big opportunity in data analytics is still to move beyond using spreadsheets,"

ANALYZING THE HUMAN ELEMENT

Advances in data analytics have enabled wide-ranging, cross-industry studies that previously would have been impossible to conduct. A recently completed project led by Texas A&M University's (TAMU; College Station, Tex.; www.tamu.edu) school of public health, in collaboration with the college of engineering, investigated the application of written procedures at several different companies' operating sites across the globe and the ramifications on process safety. The team conducted extensive interviews with numerous plant operators across multiple sites. The research led by Farzan Sasangohar, an assistant professor of industrial and systems engineering at TAMU, used qualitative data analysis (QDA) to generate hypotheses and recommendations on a broad range of topics affecting safety procedures, from the effects of weather to the provision of handheld devices. "There are many systemic issues in industry procedures that still need to be uncovered, and a lot of them are difficult to uncover because they are deep in the system's design, and they are societal or psychological," says Sasangohar. The team used a QDA method known as grounded theory, which enabled interviewees' responses to be coded and analyzed to reveal commonalities and patterns on different environmental, organizational, team and task levels. "These levels all interact. There are personal issues, there are team-level issues, organizational and societal issues, and they all interact in really complex ways. The only way to uncover these issues is to conduct a large-scale holistic study to understand the contributors to safety culture," he continued.

One pattern the work revealed is a phenomenon the team dubbed "automaticity," meaning that operators become so experienced in doing certain tasks that they complete them simply via rote repetition rather than referencing the official procedures. It is situations like this, says Sasongohar, where human error and distraction can become increasingly problematic. Another issue revealed in the study is the prevalence of a "reactive" mindset with regard to updating procedures. "Even though organizations know a problem may exist, they still do not intervene by making procedural changes until an incident actually occurs," explains Sasangohar. "There are still systematic barriers to making the 'safety first' mindset a reality. Recent advances in training for safety and human factors engineering have resulted in engineers who are more prepared and resilient at a personal level, but organizations themselves must be resilient. This does not change overnight. Systematic intervention must happen," he emphasizes.

The sheer amount of information required for this study has taken years to collect, codify and analyze, and the team believes that many more articles and recommendations will be generated from this study. According to Sasangohar, an area of opportunity in data science that will help facilitate similar studies is improving probability and risk assessment with regard to human error and decision-making. "Some of the current activities to analyze human reliability require superficial quantification of qualitative data. We try very hard to quantify risk for human decision-making and human error, but much work still remains. Multiple efforts are moving forward to address this challenge," he says. ❑

he says. He notes that while data analytics is possible using spreadsheets, it is cumbersome and more time–consuming than modern analytics software. He believes the CPI should look to the same underlying technologies utilized by more consumer-facing sectors to facilitate their data analytics, including the principles employed by large entities like Amazon, Uber and Google. "It's time to get beyond spreadsheets as the everyday tool for investigation and reporting. Using a spreadsheet to perform data analytics is like using a wrench to drive a nail."

Predicting the future with big data

A key part of effectively implementing data analytics is collecting a large enough volume of the most relevant data. "Chemical plants have used production-driven data, such as temperatures, pressures and flowrates, to manage processes for decades, but an explosion in data volumes is coming as the costs of sensors and data-acquisition systems drop, and the value of data for other functions, such as maintenance and reliability, is proven," says Bob Miller, director of predictive diagnostics at John Crane Group (Chicago, Ill.; www.johncrane.com). However, he says that most plants do not currently capture the data required to properly drive a predictive maintenance strategy. "Process data alone cannot tell the whole story about the health of an asset. Sensing and data acquisition must be a part of the solution," he points out. John Crane is currently piloting a new predictive-diagnostics platform for mechanical seals and other rotating-machinery components at several CPI facilities. The company expects a full commercial rollout of this technology in 2018. The platform features proprietary algorithms created with input from rotating-machinery experts. "The goal of our algorithms is to have enough specificity on what's going wrong to give sufficient lead time to recommend some kind of minimally invasive maintenance action to prevent failure," Miller explains. "We are selling people the knowledge of when something may fail and what can be done to prevent it." While some of the operational and safety benefits realized by predictive diagnostics may seem obvious, Miller points out that one of the most significant parameters is still overlooked. "Even the most sophisticated users may not be tracking the impact of lost production due to an unplanned failure on a routine basis," he adds.

A major challenge in implementing these types of strategies, however, is the current practice of "siloing" plant data. According to Miller, many sites will run predictive diagnostics on a single machine, rather than looking at the entire process, sometimes resulting in unexpected maintenance burdens. "Sometimes we observe that an operational decision designed to increase production in one unit can have an impact on the maintenance of a downstream unit. Bridging gaps in those data silos can unlock another level of optimization for plant operations," he states (Figure 2). Miller has observed a few market leaders in the CPI who are proactively implementing integrated data-analytics strategies. There is, however, still much work to be done in moving toward a more plant-wide model of data analytics. Miller believes that as value is proven for analytics in specific applications, more users will become receptive to integrated, overarching platforms.

In January, Black & Veatch (Overland Park, Kan.; www.bv.com) launched a new subsidiary focused on data analytics called Atonix Digital. According to Fred Ellermeier, president of Atonix Digital, the group's focus is deploying operational intelligence and adaptive planning capabilities through the Asset360 platform, a predictive cloud-based artificial intelligence system. "The big change we've seen is the openness to allow very mission-critical systems to be monitored, diagnosed and planned with cloud-based solutions," says Ellermeier. While cloud-based solutions are very powerful, people are

John Crane Group

FIGURE 2. **Next-generation data analytics should be integrated and collaborative across organizations, rather than siloed into individual equipment units**

still learning to be comfortable with data residing in the cloud. However, according to Ellermeier, through encryption and anonymization, data can be stored very securely in the cloud, and in many cases, more securely than at on-site premises.

"The operational intelligence space is becoming more crowded, but the predictive side of things is quite cutting-edge — being able to tell the future using large streams of data," explains Ellermeier. This includes being able to incorporate new streams of data — weather patterns, for instance — and overlay them with detailed historical data.

Atonix has successfully used predictive analytics for leak prevention in water-treatment sites. "We use advanced tools to predict where leaks will happen next. New adaptations in data sciences have allowed us to be able to do that," says Ellermeier. "You can begin to predict when problems are going to occur and look at how to take care of assets in a controlled manner before problems arise," he continues. Atonix has also used advanced analytics to optimize water-treament pumping stations. Work has also been done supporting analytics for waste-to-energy and combined heat and power projects. Atonix is looking to expand its footprint further into the CPI, and plans are underway to branch into the food-and-beverage market with new predictive tools.

A number of other groups from across the CPI have announced business efforts in the digitalization and analytics realm. In January, Koch-Glitsch, LP (Wichita, Kan.; www.koch-glitsch.com) entered a partnership with EFT Analytics focused on applying machine learning to enable comprehensive visibility of live plant operations for refining and petrochemical plants. BASF SE (Ludwigshafen, Germany; www.basf.com) invested in startup company Ahrma Holding B.V. to accelerate analytics-based logistics and supply-chain capabilities. Last year, thyssenkrupp Industrial Solutions (Essen Germany; www.thyssenkrupp-industrial-solutions.com) began offering data-based services to the mining sector, including a nearly universally compatible radar technology to perform online, realtime measurements. SUEZ (Paris, France; www.suez-environnement.fr) recently introduced a cloud-based, analytics-driven asset management system with geomapping technology for water-treatment sites. These are surely only a fraction of the analytics efforts coming down the CPI pipeline in the coming months. ■

Mary Page Bailey

Improving the Daily Grind

New milling, grinding and size-eduction equipment helps processors obtain better efficiencies and develop new products

IN BRIEF

INCREASING EFFICIENCIES

EXTENDING TO BROADER AREAS

PROCESSING SPECIALTY PRODUCTS

SMALLER PARTICLES

'GREEN' MARKETS

Although milling and size-reduction equipment may be mature — some technologies date back to the 1800s — evolving needs of chemical processors, including the demand for better efficiency, new applications and materials and other trends, require milling and size-reduction equipment manufacturers to constantly innovate. Here's a look at what's new in modern milling and size-reduction equipment, as well the driving forces behind today's offerings.

FIGURE 1. Due to the improved process control of the MacroMedia (left) in the pre-grinding stage, fluctuating raw material qualities can be balanced out, achieving uniform properties for intermediate products, allowing an optimization of the fine grinding process with the MicroMedia bead mill (right)

"We work hard at improving our products and are still coming out with new and patented features that add value for our customers," says Chris Nawalaniec, vice president of sales and marketing with Stedman Machine (Aurora, Ind.; www.stedman-machine.com). "Everything we do today targets improving either product quality, lowering operating costs or designing a new process for our customers to help optimize their specific projects. We study different metallurgy for wear parts and use computational fluid dynamics (CFD) to model material flow through machines so we better understand where we need to improve parts from a wear standpoint and equipment from an energy-consumption standpoint. We've had success in terms of coming out with feature improvements that help customers."

Increasing efficiencies

Energy and space efficiency are some of the most crucial considerations when chemical processors seek milling and size-reduction equipment, and mill providers are responding in a variety of ways.

Bühler AG (Uzwil, Switzerland; www.buhlergroup.com), for example, is offering a solution for wet grinding that includes the MacroMedia pre-dispersing unit and the MicroMedia bead mill, says Norbert Kern, director of product management and process engineering at Bühler. The combination of the pre-dispersing unit for pre-conditioning with the bead mill for fine grinding and fine conditioning of material results in higher-quality product in a shorter period of time, with less energy consumption.

Due to the improved process control of the MacroMedia (Figure 1, left) in the pre-grinding stage, fluctuating raw material qualities can be balanced out, achieving uniform properties for intermediate products, allowing an optimization of the fine grinding process with the MicroMedia bead mill (Figure 1, right). "Our bead mills employ beads that are used to grind the product into smaller sizes. Using smaller beads in the same size grinding machine allows more contact points and

Air Products

FIGURE 2. Air Products' PolarFit cryogenic grinding technology uses liquid nitrogen to super-cool the materials being ground, which temporarily changes the physical properties of difficult- or impossible-to-grind materials, making them easier to grind

Hosokawa

FIGURE 3. Hosokawa's Mikro UMP Universal Milling System, a compact, high-speed impact mill, is capable of coarse granulation or fine size reduction thanks to interchangeable rotor configurations. The system provides the same grind as a traditional hammer-and-screen setup while adding the flexibility of converting to a pin mill for fine size reduction or a rigid rotor for de-agglomeration

more efficient grinding, resulting in faster throughput and improved quality levels," says Kern.

Not only does this create more efficiency in the grinding process itself, but the use of smaller beads also boosts energy and space efficiency because less energy is required to achieve higher output performance in the same equipment footprint, explains Kern.

Extending to broader areas

While material size reduction has long been an integral unit operation in the chemical process industries (CPI), there is growing interest in the processing of heat- or oxidation-sensitive and impact-resistant materials. Examples of these include nutraceuticals and pharmaceuticals or tough polymers used in 3-D printing and powder coatings. These emerging, high-tech materials present size-reduction challenges that can be addressed by Air Products' PolarFit cryogenic grinding technology (Figure 2), which uses liquid nitrogen to super-cool the materials being ground.

As Tim Boland, principal equipment engineer with Air Products (Lehigh Valley, Pa.; www.airproducts.com), explains, "Processors may be dealing with materials that are difficult or impossible to grind in an economical fashion using traditional, ambient-temperature grinding technology. With cryogenic grinding, liquid nitrogen is used to super-cool these materials and temporarily change their physical properties, making them easier to grind."

Another advantage of using liquid N_2 in cryogenic grinding is the generation of inert N_2 gas. "Any time you process combustible materials there is the potential for a dust explosion. Nitrogen gas, either generated during cryogenic grinding or intentionally introduced as a gas into the solids processing equipment, helps mitigate the risk of dust explosions," Boland says.

Processing specialty products

While the trend had been for U.S. manufacturing and processing industries to move overseas in an effort to compete on a cost basis, during the past five or six years, the cost of production in many overseas countries began to rise, bridging the cost gap and causing a shift in some processing back to the U.S. "While it is still more expensive to manufacture in the U.S, it is closer in cost than it had been. Currently, a lot of U.S.-based processors are bringing production of specialty, higher-value products back to the states. However, they need to do so in a more efficient manner," says Bill Brown, director of sales and marketing with Hosokawa Micron Powder Systems (Summit, N.J.; www.hmicronpowder.com). "To meet this need, we added more sophisticated controls so less human interface is required, increased process efficiency of the milling and classification systems and fine-tuned these processes for tighter, more efficient control of airflow to reduce energy consumption."

In specialty product processing, providing systems that address efficiency needs, as well as versatility, is a necessity. Hosokawa's Mikro UMP Universal Milling System, a compact, high-speed impact mill capable of coarse granulation or fine size reduction with interchangeable rotor configurations, fits the bill (Figure 3). The system provides the same grind as a traditional hammer-and-screen setup while adding the flexibility of converting to a pin mill for fine size reduction or a rigid rotor for de-agglomeration.

While the system provides flexibility across the food, pharmaceutical and chemical industries, one of the latest applications for this technology is in polymers and plastics. "Processors are producing polymers down to 30-, 40- and 50-mesh particle sizes and often produce a wide range of materials, which requires frequent changeovers," notes Brown. "This milling system allows them to get a smaller and finer product and quickly change rotors out to produce differ-

Fritsch

FIGURE 4. Fritsch's Planetary Mill Pulverisette 5 premium line features two grinding stations for fast wet and dry grinding of hard, medium-hard, soft, brittle and moist samples, as well as for mechanical alloying, mixing and homogenizing of larger sample quantities with reliable results down to the nanometer range

ent materials, which means they can get into new markets and sell products of a much higher value into specialty applications at a higher profit."

Smaller particles

A decade ago, laboratory milling process capability ended somewhere with particles in the micrometer range, but, recently, the need for smaller particles is growing. "Everyone wants to know how fine we can get with our particles, with customers requesting sizes into the nanometer range," says Wolfgang Simon, sales director with Fritsch International (Idar-Oberstein, Germany; www.fritsch-international.com).

The interest in nanomaterials, says Simon, is because, as particles get smaller, they have completely different physical and chemical properties. For example, in the solar cell industry, if zinc oxide is milled into the nanometer range, it changes from a yellow powder to a transparent powder, yet retains the same electrical properties, allowing users to coat a solar cell with this clear nano-powder and maintain the electrical properties needed to conduct the electricity. And, in the pharmaceutical industry, the finer the active pharmaceutical ingredient (API), the lesser the amount of substance required. "When the API is in the finer nanometer range, the effects inside the body will be faster, meaning you need less active API for the same result and with less side effects," explains Simon.

And, getting to the nanometer range on a laboratory scale is of utmost importance in research and development (R&D) of new products, such as those for lithium ion batteries and medicinal cannabis, according to Simon. However, while smaller particle sizes are a growing trend in R&D, mills capable of producing smaller particles must still be viable for daily use in the laboratory. This means they must be as safe, efficient and easy to clean as mills designed to produce larger particle sizes. To satisfy this need, Fritsch developed its Planetary Mill Pulverisette 5 premium line with two grinding stations for fast wet and dry grinding of hard, medium-hard, soft, brittle and moist samples, as well as for mechanical alloying, mixing and homogenizing of larger sample quantities with reliable results down to the nanometer range (Figure 4).

The mill works on the planetary principle, which employs the high-energy impact of grinding balls, as well as friction between grinding balls and the grinding bowl wall. The grinding bowl, containing the material to be ground and grinding balls, rotates around its own axis on a main disk rotating in the opposite direction. At a certain speed, the centrifugal force causes the ground sample material and the grinding balls to bounce off the inner wall of the grinding bowl, cross the bowl diagonally at an extremely high speed and impact the material to be ground on the opposite wall of the bowl. The grinding bowls reach twice the speed of the main disk during this process. Due to the 2.2-kW drive power and centrifugal acceleration, high-performance grindings down into the nanometer range are possible.

Smaller particles are also frequently requested on the process scale, where a balancing act between ultrafine grinding and energy efficiency is often a challenge, according to Peter M. Koenig, product manager for particle processing at Bepex International LLC (Minneapolis, Minn.; www.bepex.com). "There's been a shift in the process industry to get finer and finer grinds. In addition to smaller particles, users also want the particles created specifically for their end use. This means they don't want them finer than they have to be and they want to control the top size, as well, which requires controlling the overall distribution."

However, the desire for reduced and specific sizing can have consequences on energy efficiency. Achieving smaller-sized particles requires a higher impact velocity, necessitating more energy; conversely, if less energy is used to fracture the particle, it may be necessary to run materials through multiple times, ultimately using more energy. "With this in mind, we strove to produce a finer particle at a lower impact velocity," he says.

Bepex

FIGURE 5. Bepex's Pulvocron Air Swept Pulverizer provides high-speed material impact and internal classification for ultrafine grinding of powders and cakes. It is well suited to applications requiring moderate moisture reduction and fine size reduction in a single step

While the equipment Bepex developed does not reach the nanometer range, the Pulvocron Air Swept Pulverizer (Figure 5) provides high-speed material impact and internal classification for ultrafine grinding of powders and cakes. It is well suited to applications requiring moderate moisture reduction and fine-size reduction in a single step. The short residence time and intense milling action inside the chamber offer high-efficiency processing of the material in a compact system.

"We can achieve and control very high impact velocities, as well as the tolerance between the impact surface and the liner, which prevents bypassing of coarser particles," explains Koenig. "These very tight tolerances at high impact speeds allow the equipment to grind both crystalline materials that shatter on impact, as well as tough materials that require shredding. On exit, the material goes through an air classifier, which, by centrifugal speed, performs separation of fine and coarse materials. Coarse materials are reintroduced to a return stream and back to the mill, while the fine classified material is collected."

This system not only provides ultrafine grinding, but also boosts energy efficiency because only material that is too coarse gets reintroduced. "We grind only the parts that need grinding, so it can produce more product on specification at lower energy consumption," Koenig says.

'Green' markets

There is a big push for green, sustainable and landfill-free processing, according to Steve Knauth, marketing and technology manager with Munson Machinery (Utica, N.Y.; www.munsonmachinery.com). "We are seeing the trend toward recapture and reuse accelerate among our customers," he says. "In addition, they are also looking for equipment that is going to minimize the amount of material that must be sent into the atmosphere or landfill. This means processors need size-reduction equipment that can handle these green applications while producing less fines."

As a result, Knauth says his company is seeing a shift away from hammer mills and toward the company's SCC Screen Classifying Cutter in many applications, because it's designed to reduce hard and semi-hard particles into fairly precise sizes. It is also easily controllable, which means it produces less fines, reducing the amount of material captured in the dust collection system.

The SCC Cutter performs like a knife cutter, but handles a greater diversity of materials, including friable, semi-friable, fibrous, semi-hard and hard materials, and retains sharpness. At medium to high speeds, it impacts material similar to a hammer mill, but adds the flexibility of variable speed for greater control of particle sizes. The rapid throughput with less impact results in minimal fines. "All this lends itself well to the green industry trend. The SCC Cutter is capable of recapture and reuse/recycle applications due to the variety of materials it can handle, and minimal fines means there is less material in the dust collection system for disposal," notes Knauth. ■

Joy LePree

Focus on Motors and Drives

IDEC

New line of stepper motion-control products released

This product line includes controllers, stepper motors, an integrated controller/drive, an integrated drive/stepper motor, and an integrated controller/drive/stepper motor (photo). The integrated controller/drive and drive/stepper motor units save space and money, and simplify installation, by combining multiple components into a single unit. The integrated controller/drive/stepper motor units offer space savings, cost effectiveness and system simplification. As compared to more complex servo-motion control systems, steppers are a simpler technology, and require no tuning or adjustment. They also have excellent torque at low speeds, don't require position feedback, and have very low maintenance requirements, says the company. These characteristics make them a suitable fit in a variety of applications, including pharmaceutical, printing, packaging, material handling and semiconductor industries. — *IDEC Corp., Sunnyvale, Calif.*

us.idec.com

Electric Torque Machines (ETM)

Smaller motor for pumps improves performance

This company has recently extended its focus on motor applications to include positive displacement pumps. Peristaltic pumps require relatively high torque at low rotational speeds, typically in the range of 5 to 500 rpm, well below the direct-drive capability for incumbent, conventional a.c. or d.c. motors. As a result, incumbent motors are operated at a higher speed (over 1,000 rpm) and a speed-reduction gearbox is necessary to achieve the required torque and rotational speed. As a result, these geared-drive systems can be large, heavy and inefficient. Also, the gearbox increases cost, while causing a reliability and maintenance burden. Compared to these conventional geared systems, the direct-drive motors deliver high continuous torque at low rotational speeds, which eliminates the need for a speed-reduction gearbox and reduces the drive system size and weight (photo). The motors use transverse flux technology with increased pole count and low resistance coils, delivering 5–10 times more continuous torque by mass compared to conventional a.c. or d.c. motors. And, according to the company, compared to the a.c. geared system, power consumption versus pump speed is reduced 29–54% for the direct-drive system. — *Electric Torque Machines (ETM), Flagstaff, Ariz.*

www.etmpower.com

PI

Motor stage family with direct drive offers new options

This company expanded its PIMag series of linear motor stages with the V-508, a new series of compact linear-positioning stages with high force three-phase linear motors and crossed roller guides (photo). The V-508 family of linear motor stages is offered with 80-, 170-, and 250-mm travel range. Two motor options are available: ironless for highest resolution and smoothest motion; and iron-core for highest force, acceleration, and velocity up to 1 m/s. Mechanically, the V-508 series features high-load, precision crossed roller bearings with anti-creep cage assist, preventing roller creep, which allows a long lifetime in high-duty cycle industrial applications, together with the zero-wear, non-contact linear motor. Linear motors provide smooth motion, and a high dynamic velocity range along with rapid acceleration, because they provide motion directly without the need of additional mechanical components, such as drive screws and gearboxes that add friction, vibration and noise. They are well-suited for scanning applications or automation tasks where repetitive fast start-stop motion with high precision is required and where reliability and maximum uptime are crucial. In addition to electromagnetic three-phase and voice-coil linear motors, this company also provides several types of electro-ceramic linear motors. — *PI, Auburn, Mass.*

www.pi-usa.us

Note: For more information, circle the 3-digit number on p. 62, or use the website designation.

Monitor vibration levels for predictive maintenance

Cloud-based computerized maintenance management software (CMMS) has been introduced by this company to integrate sensors to measure temperature and vibration levels of equipment, such as motors, gear boxes and more. Adding these smart sensors (photo) provides users with realtime data for condition monitoring through which alerts can be viewed directly from the CMMS dashboard. The CMMS works from both desktops and mobile devices. A simple screw-type mounting design can be used for the sensors. — *EZmaintain, Elyria, Ohio*
www.ezmaintain.com

Manage motors via several communication options

The Simocode pro motor management system (photo) for motor monitoring and control has been expanded to incorporate new communication connectivity. Alongside the existing options over Profinet, Profibus and Modbus, open communication over EtherNet/IP, including additional EtherNet-based services such as NTP (network time protocol) are additionally available. The motor control devices of the Simocode pro product series were developed specifically for the management of motors in the low-voltage range. The system operates independently of the controller and offers protection, monitoring, safety and control functions between the motor feeder and the automation system. Because the EtherNet/IP communication protocol is provided on the individual communicating device, no additional communication devices, such as protocol converters, or adapters are required. — *Siemens AG, Munich, Germany*
www.siemens.com

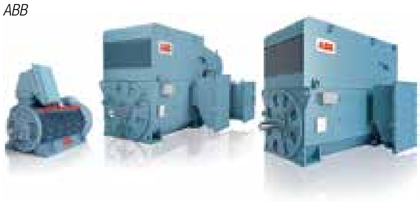
These general purpose motors meet most needs

The N-series general purpose motors (photo, p.22) provide energy efficiency, reliability and safety in applications where a highly customized motor is not needed. The motors use

EZmaintain

Siemens

ABB



cost-effective pre-packaged designs with short lead times. N-series motors currently include three product families: the high-voltage rib-cooled and modular-induction motors, and a new range of slip-ring motors. Even in their basic configuration the N-series motors satisfy most common requirements in many industries. A number of pre-engineered option packages are available. Vertically mounted motors fitted with thrust bearings, for example, are widely used in pumping applications. — *ABB, Zurich, Switzerland*
www.abb.com

This speed reducer fits IEC or NEMA motors

The FlexFrame 5-hp face-mounted speed reducer (photo) incorporates patented adaptors that allow it to be used with either IEC or NEMA motors. Users can quickly switch or replace motors, interchange IEC and NEMA motors for export applications, add face, flange or foot mounts, and use shaft adaptors to match virtually any motor to any gearbox. Consisting of a face-mounted speed reducer with a hollow shaft input, these new designs function as gearheads. They are available in standard ratios of 3:1, 4:1 and 5:1, making them suitable for a wide range of industrial and commercial applications, including use on mixers, conveyors, hoists and other material handling equipment, food processing equipment, robotic drives, and more. With aluminum housings, FlexFrame units are lightweight with a small profile, creating a premium weight to torque ratio (power density), says the company. — *Gearing Solutions, Solon, Ohio*
www.gearingsolutions.com

Gearing Solutions

New compact ring drive has a built-in brake

The new compact ring drive (CRD) system, CRD 250B (photo), includes a built-in zero-backlash locking brake design that delivers twice the nominal torque without increasing the CRD footprint. It is durable, with a brake life of one million cycles, and requires little maintenance. The brake is spring engaged and pneumatically released so that it will default to lock in a power-failure or emergency situation. The CRD has a precision-grade bearing and drive mechanism in sealed housing. The three-drive design configurations allow it to be optimized for high speeds of up to 225 rpm, high torque or both. — *Nexen Group, Inc., Vadnais Heights, Minn.*
www.nexengroup.com ■

Nexen Group

Dorothy Lozowski

New Products

New software features for CFD, thermodynamics and more

Version 5.3a, the latest release of this company's Multiphysics software (photo), provides many enhanced simulation capabilities for users of computational fluid dynamics (CFD) analysis, including up to 40% improved performance for algebraic multigrid (AMG) and 20% for geometric multigrid (GMG) solvers, says the company. Chemical engineers will benefit from the built-in library for thermodynamics properties, which features models for gases, liquids and phase equilibria (gas-liquids). Furthermore, there is a new turbulence model available for a more accurate description of fluid-flow features. A predefined multiphysics coupling has been introduced for the modeling of heat and moisture transport in materials and moist air. The software also features the Cividis color table, which is optimized for people with color-vision deficiency (photo). Applications with very large plots or many graphics windows will see improved rendering performances, resulting in a more responsive user interface. — *Comsol, Inc., Burlington, Mass.*
www.comsol.com

A conductivity meter designed especially for CIP systems

The CombiLyz conductivity meter (photo), with an accuracy of ±1% and a measuring range of 500 µS/cm to 1,000 mS/cm, together with robust temperature compensation, provides many important features for clean-in-place (CIP) systems. Where CIP systems require acids or alkalis, accurate measurement of concentration levels is essential. While the concentration of the acid or alkali is increasing, the conductivity meter controls the specified concentration of the relevant cleaning media. The meter's precise measurements ensure that no excess chemicals are used. During the phase separation in the CIP return flow, the CombiLyz quickly recognizes different media, even when temperatures fluctuate significantly, helping to reduce the loss of stored cleaning agents. After one cleaning cycle, the CombiLyz accurately measures the concentration of the remaining chemicals in the rinse water. With this information, the programmable logic controller (PLC) can control the predefined media circuits using valve nodes, reducing the risk of contamination by residual chemicals. A compact design reduces flow resistance in the process line, and deposits and impurities can be easily flushed out of the system. — *Baumer Ltd., Swindon, U.K.*
www.baumer.com

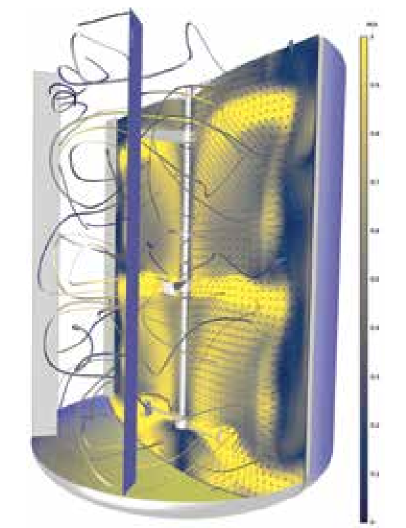
Embedded anomaly detection improves cybersecurity

This company's Open Secure Automation (OSA) products (photo) will now include intrinsic anomaly detection (AD) as standard integrated functionality that continuously monitors the controller's network and system time to detect intrusions and abnormal behavior. The AD system includes dynamic port-connection monitoring, which records all attempts to connect any controller or communication point and captures identifying information on the intruder, as well as network port scanning, which detects if hackers are scanning for open ports that might provide access to the control network. System time is also monitored to detect attempts to manipulate log files to conceal malicious activity. A cryptographic engineering key lock permits only users with valid user credentials to change the configuration and operation mode of the controller. The AD system also logs all detected anomalies and exports them for historian, alarming and trending functions. — *Bedrock Automation, San Jose, Calif.*
www.bedrockautomation.com

Effectively remove air, gas and water vapor from many materials

The MV benchtop vacuum-degassing chamber (photo) is constructed from 304 stainless steel with a pump-out port, isolation valve, vent valve and vacuum gage, as well as an inlet trap to prevent damage to the vacuum pump from vapors. Featuring a clear Lucite top for interior viewing, it rapidly removes entrapped air, gas and water vapors from a variety of materials. Available in 15- and 4-gal sizes, the MV vacuum degassing chamber can be supplied with rotary motion feed-

Comsol

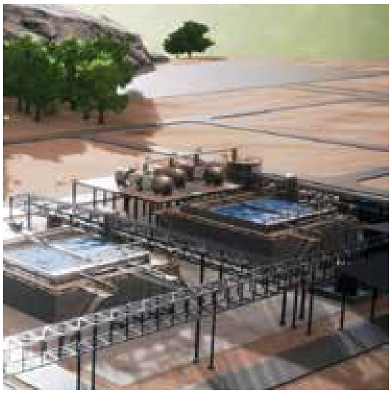


Baumer

Bedrock Automation

Mass-Vac

Outotec



Hospeco

Vortec

Endress+Hauser

throughs, shelves or other accessories, and can be custom designed to user specifications. This versatile system is capable of operating at pressures up to 0.5 Torr and can be supplied with or without vacuum pumps with capacities ranging from 5 to 20 ft^3/min. — *Mass-Vac, Inc., North Billerica, Mass.*
www.massvac.com

More sustainable water management for mining

This company's Process Water Recycling Plant (photo) is a fully automated standalone unit that enables recycling of process water from mining operations. The plant is specifically designed for concentrator plants, which dewater tailings and recycle the water back to the process. It enables undisturbed process performance by treating recycled water and removing accumulated substances to achieve the desired level of quality for the various duty points of the concentration process. Because the plant is modular and based on predesigned treatment units, it is fully configurable for each individual process. A full range of complementary services are available, including process assessment, laboratory- and pilot-scale testing and analysis, technical studies and remote monitoring and support. — *Outotec Oyj, Helsinki, Finland*
www.outotec.com

Protect against slips and falls with these absorbent floor mats

TASKBrand SureGrip absorbent adhesive floor mats (photo) feature next-generation sorbent technology to help prevent slips, trips and falls and protect floors from moisture with impermeable adhesive backing. The mats are fast-drying and can be easily custom cut for hard-to-fit areas. The heavyweight, universal sorbent material absorbs excess moisture, oils, greases, condensation and other spills. SureGrip is also an effective barrier protection, stopping dust, dirt and debris from entering enclosed spaces. The adhesive backing assures the floor covering stays in place, even with constant foot traffic or rollover by wheeled equipment. The mats can be swept, vacuumed, mopped or cleaned with floor scrubbers or shop vacuum cleaners. — *Hospeco, Cleveland, Ohio*
www.hospeco.com

Air-conditioning vests improve comfort in extreme environments

Working in extreme environments can take a toll on workers, but these dual-action personal air conditioners (PACs; photo) keep workers comfortable in either hot or cold working conditions. PACs minimize heat stress and fatigue in elevated temperatures, or with simple adjustment, they raise vest and body temperatures to ward off the cold. A dual-action PAC generates cold or hot air to provide airflow to the worker, along with a cooling/heating vest that diffuses the air flows around the worker's torso. They do not restrict movement, do not absorb sweat or other contaminants, and can be worn under other protective clothing. When wearing PACs, workers require fewer and shorter cooling and warming work breaks, increasing overall productivity. Tubes convert compressed air to a low-pressure cold or warm air source. A compressed air stream enters the vortex tube where it spins rapidly, splitting into hot and cold air streams. — *Vortec, Cincinnati, Ohio*
www.vortec.com

Use this tablet to connect almost any field device

The Field Xpert SMT70 (photo) is a rugged tablet for commissioning and maintenance staff that manages field instruments and documents the work progress. The tablet comes pre-installed with the DeviceCare device configuration software and device library. The Field Xpert can connect to field instrumentation devices directly via a USB or Bluetooth wireless modem, or via a gateway, remote I/O or multiplexer to a bus system. The Field Xpert device library has more than 2,700 pre-installed device and communication drivers, allowing it to work with many different instruments from a wide variety of vendors. The drivers can be used to communicate with virtually all HART and Foundation Fieldbus devices, and additional device drivers can be installed if required. The battery runtime is 14 h. The tablet comes in a general-purpose configuration as well as a hazardous-area configuration. — *Endress+Hauser Inc., Greenwood, Ind.*
www.us.endress.com/SMT70 ■

Mary Page Bailey

Flow Measurement in Large Lines, Ducts and Stacks

Department Editor: Scott Jenkins

Process industry plants install sophisticated air-pollution control systems, but they can be ineffective if the flowmeters on which they rely deliver inaccurate or unreliable data. This one-page reference provides information on measuring the flow of gaseous combustion products in large pipes, ducts and stacks.

Flue products

A flue is typically a large pipe, duct, stack, chimney or other venting apparatus attached to an industrial plant system, such as a boiler, furnace, steam generator or oven, through which waste gases are exhausted. Depending on a number of factors, including the type of industrial plant, process characteristics, fuel used and efficiency, fluegases can include the following compounds:

- CO_2
- CO
- CH_4
- N_2
- NO_x
- O_2 and H_2O
- Ozone
- Sulfur oxides
- Particulate matter

Environmental standards

For large stack-monitoring applications, the U.S. Environmental Protection Agency (EPA) requires a continuous emissions monitoring system (CEMS) or rate monitoring system (CERMS). For CERMS, the flowmeters must perform an automated and on-demand self-checking of calibration drift (CD) at both a low-range and a high-range flow point.

In the E.U., these systems are referred to as automated measuring systems (AMS). The flowmeters that support them also need to meet the quality assurance level 1 standard, confirming compliance to EN 15267-1,-2,-3 and EN 14181 standards.

Measurement

Measuring the flow of stack- or fluegas is a challenge (Figure 1). Fluegases are generally of mixed composition, and the volume emitted varies based on the products of the process, workload schedules and seasonal temperature and humidity fluctuations. This variability can lead to irregular swirling flows that are difficult to measure without multipoint sensing.

Large-diameter pipes, stacks and ducts present unique physical challenges to successful flowmeter installation and performance. Installations are complicated by difficult-to-reach access points, single-plane platforms, long cable runs, extra mechanical support and exposure to weather extremes.

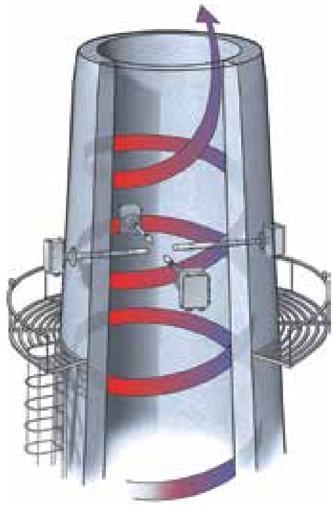


FIGURE 1. The composition of fluegas is mixed and the volume varies depending on products, workload and weather

Lack of pipe straight-run, distorted flow profiles, low flowrates and wide turndown rates are common performance challenges for many flowmetering technologies. Furthermore, the gas can be dirty and at high temperatures, which can result in measurement degradation, clogging and fouling that lead to excessive maintenance procedures or premature flowmeter technology failures.

Gas flow measurement is increasingly a multipurpose endeavor: objectives are to ensure compliance with government regulations and to provide data on process gases for scrubbers and flare systems. The combination of these factors results in the need for flowmeters that operate accurately and reliably over a wide flow range in rugged environments with distorted and swirling flow profiles.

Evaluating technologies

In considering flowmeters for gas monitoring, the first step is to choose the appropriate flow technology. Several flow-sensing technologies are available, including the following: Coriolis (mass); differential pressure; electromagnetic; positive displacement; thermal (mass); turbine; ultrasonic; and vortex shedding. These technologies all have advantages and disadvantages depending on the type of process fluid (air/gas or liquid). Process engineers must consider many factors, such as limited straight-run challenges, dirt and particulate matter, mechanical installation, high temperatures and moisture entrained in the flow stream, in addition to cost-benefit considerations in meeting accuracy requirements, maintenance and life expectancy of the equipment.

Looking at these factors, along with the plant's layout, environmental conditions, maintenance schedules, energy cost and return on investment (ROI), will narrow the field. The most common flow-sensing technologies chosen for fluegas measurement are differential pressure (averaging Pitot tubes) flowmeters and thermal dispersion mass flowmeters. Both technologies have similar accuracy levels when configured with multiple sensing points within the large cross-sectional area of a fluegas line. For swirling flows of hot fluegases, multipoint sensing generally provides more accurate flow measurement than single-point technologies.

Maintenance requirements, which raise operating and lifecycle costs while reducing return on investment, are different for the two technologies. Most averaging Pitot tube flow sensors require a daily manual or compressed-air backpurge system to keep the inlets from clogging. Thermal flowmeters, with no inlets or moving parts, can require virtually no maintenance for years.

Examining the accuracy, installed cost and lifecycle cost of the various flow-sensing technologies available for fluegas monitoring allows an informed selection of equipment. Unique problems may benefit by consulting flowmeter suppliers. ■

Editor's note: The content for this edition of "Facts at your Fingertips" column was initially prepared by Steve Craig, a senior member of the technical staff at Fluid Components International (FCI; San Marcos, Calif.; www.fluidcomponents.com).

Cyclohexane Production from Benzene and Hydrogen

By Intratec Solutions

Cyclohexane is a relatively stable cycloalkane, present in crude oils in concentrations of 0.1–1.0%. This cycloparaffin is a colorless, flammable liquid, widely used as an intermediate in nylon manufacturing. On a commercial scale, cyclohexane production is almost entirely based on the catalytic hydrogenation of benzene, which can be conducted in the liquid or vapor phase in the presence of hydrogen.

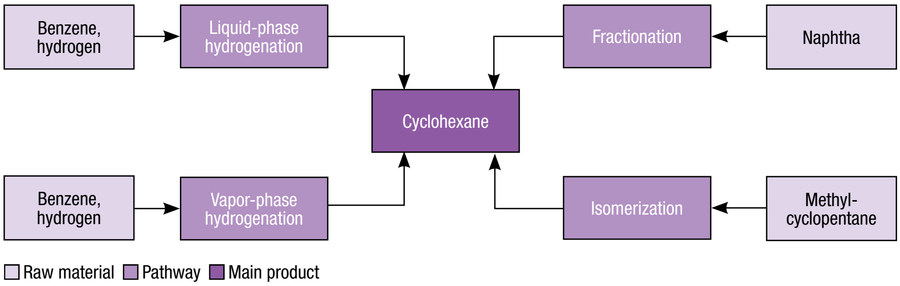


FIGURE 2. Several production pathways exist for producing cyclohexane

The process

The following paragraphs describe a process for the production of cyclohexane from benzene and hydrogen that involves liquid-phase hydrogenation of benzene in the presence of a nickel-based catalyst. Figure 1 presents a simplified flow diagram of the process.

Reaction. Initially, benzene is fed to the primary reactor along with fresh and recycled hydrogen. The hydrogenation reaction is carried out in a bubble column reactor, in the presence of a nickel catalyst. The catalyst is maintained in a suspension with the aid of an external circulation loop. Most of the heat of reaction is removed by the vaporization of the product stream, which is further recovered via a top stream within the reactor. The remaining reaction heat is removed in the external loop, by passing the reactor reflux stream through a heat exchanger against boiler feedwater, producing low-pressure steam.

Most of the benzene feed is converted in this step. The top gaseous product stream is directed to a fixed-bed reactor, where the remaining benzene content is converted to cyclohexane. The finishing hydrogenation reaction is conducted in the presence of a solid nickel-based catalyst supported on alumina.

Hydrogen recovery. The product stream is fed to a knock-out drum operated at high pressure. Most of the cyclohexane in the feed condenses, producing two streams: one gaseous hydrogen-rich stream and a liquid cyclohexane-rich stream. The hydrogen stream is routed to the recycle compressor, where it is compressed to the pressure of the primary reactor and recycled.

Purification. In a distillation column, the liquid cyclohexane-rich stream that is recovered is stripped of lighter contaminants, such as methane, ethane and soluble hydrogen. Light-ends recovered from column's top are used for fuel, while a cyclohexane stream with a residual benzene content lower than 100 ppm is obtained from column's bottom.

Production pathways

Cyclohexane has been primarily manufactured by the hydrogenation of benzene, which can be carried out in both liquid and gaseous phases, in the presence of different metal-based catalysts. This chemical may also be obtained from naphtha fractionation, or by isomerization of methylcyclopentane. Different pathways for cyclohexane are presented in Figure 2.

Economic performance

The total operating cost (raw materials, utilities, fixed costs and depreciation costs) estimated to produce cyclohexane was about $1,400 per ton of cyclohexane in the first quarter of 2014. The analysis was based on a plant constructed in the U.S. with capacity to produce 200,000 metric ton per year of cyclohexane.

This column is based on "Cyclohexane from Benzene and Hydrogen – Cost Analysis," a report published by Intratec. It can be found at: www.intratec.us/analysis/cyclohexane-production-cost. ■

Edited by Scott Jenkins

Editor's note: The content for this column is supplied by Intratec Solutions LLC (Houston; www.intratec.us) and edited by *Chemical Engineering*. The analyses and models presented are prepared on the basis of publicly available and non-confidential information. The content represents the opinions of Intratec only. More information about the methodology for preparing analysis can be found, along with terms of use, at www.intratec.us/che.

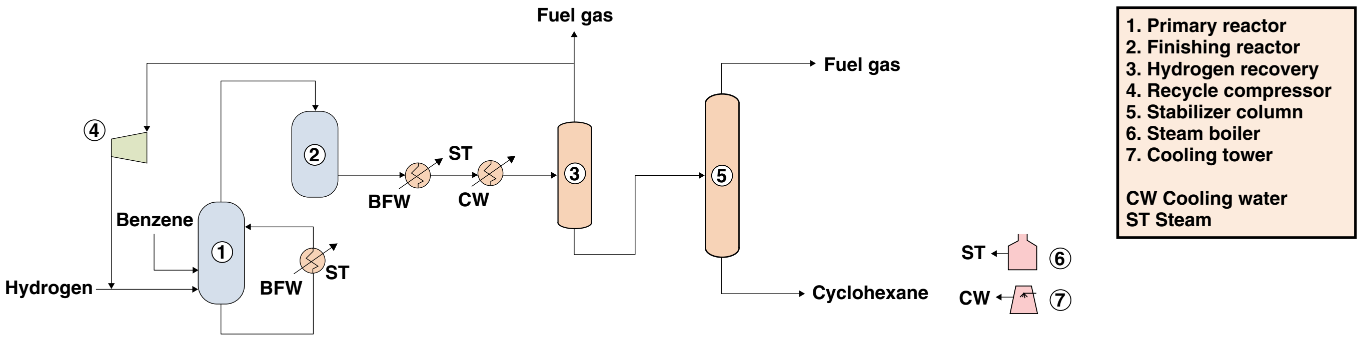


FIGURE 1. This flow diagram shows a process for producing cyclohexane

Distillation, Part 1: Experimental Validation of Column Simulations

A practical look at the need for validation, as well as conceptual considerations and a case study

Glenn Graham, Pratik Pednekar and Don Bunning
MATRIC

IN BRIEF

DIFFICULTIES ASSOCIATED WITH SIMULATIONS

CONCEPTS FOR EXPERIMENTAL VALIDATION

A CASE STUDY

This article addresses the need for experimental validation of computer-generated simulations of distillation columns, and discusses the main concepts involved with experimental validation. Also included is a case study of a simulation effort that initially yielded some uncertainties. These uncertainties were readily resolved with batch laboratory testing.

Difficulties

Potential problems with physical property models. Process simulation tools, such as Aspen Plus, CHEMCAD, and Pro-Sim Plus, are indispensable for the design and optimization of separation schemes involving distillation columns. However, the accuracy of their predictions depends highly on the physical property models used in the simulation, and it is not unusual to obtain significantly different simulation results when using different physical property models. Some level of experimental testing is often necessary to validate the simulation results.

The physical property models consist of pure component properties, thermodynamic equations and component-interaction parameters used within the thermodynamic equations. Accurate values for the pure component properties and the interaction parameters, and the correct thermodynamic equation are seldom known at the beginning of a simulation effort.

Some software packages offer built-in pure-component-property libraries containing data for various components. In these libraries, the parameters — such as those in the Antoine equation — are regressed from built-in experimental data. The user must determine if the conditions of the simulation are close enough to the conditions of the source data to allow the data to be confidently utilized. If not, literature data may be available at the conditions of interest to allow regression and estimation of new property parameters.

There are numerous thermodynamic equations that can be used to predict the vapor-liquid equilibrium (VLE) or liquid-liquid equilibrium (LLE) between various components. The differences in the various thermodynamic equations may be subtle and the selection of the most appropriate equation may not be obvious. The thermodynamic equation selection is often based on rule-of-thumb techniques. Other times, the simulator default equation can be used, or the equation may be obtained from similar simulation work in the literature, which may not have been validated. The interaction parameters between the various components that go into the thermodynamic equation are often not available in the simulation software for all of the binary pairs of chemicals. These interaction parameters often must be obtained from literature or estimated using group contribution methods like UNIFAC (universal quasichemical functional group activity coefficients) or developed from new experimental testing.

Knowledgeable and experienced engi-

neers can generally make good decisions in the selection of the thermodynamic equation and the determination of the interaction parameters when compiling the physical property models. Nevertheless, uncertainty in the reliability of the simulation results often remains. It is critical that these difficulties and uncertainties are properly considered in the development of the physical property model to avoid distillation columns that fail to accomplish the required separation, or columns that are overdesigned and incur unnecessary costs. Lack of information about the process chemicals (especially in the case of new chemicals) and their interactions lead to uncertainty in the reliability of the predictions. Experimental distillation testing is recommended, either to verify the quality of the simulation results, or to provide data to allow the physical property models to be calibrated to the subject process conditions.

Difficulties not captured by simulations. Unexpected column chemistry may also occur, generating troublesome byproducts. These byproducts may cause product-quality problems or build up in the separation system, negatively affecting the process in other ways. If the byproduct is an intermediate-boiling compound, it may concentrate in the middle of the column, and could significantly affect the known separations within the column. An example of this "bulge" effect is shown in Figure 1. The main feed to the column in this example is methanol and heptanol, which can be easily separated. If, however, a small amount of butanol, representing an intermediate-boiling byproduct, is fed to the reboiler, the butanol accumulates in the middle of the column and its concentration builds up to very high levels within the column. This accumulation of an intermediate-boiling species would cause significant changes to the separation within the column and would dramatically affect the temperature profile and the temperature sensor(s) used for control.

Other problems that cannot be predicted by simulation include foaming and fouling. Foam generation can reduce the capacity of a distillation column. In severe cases, foaming will make the column completely non-operational. Fouling of contactor surfaces may reduce the column's capacity and could affect the efficiency of the contactor.

The case for experimental validation. These uncertainties associated with the physical properties, as well as the potential for the other issues that simulations do not address, dictate that empirical testing of distillation simulations be considered (a case study demonstrating the need for experimental validation of simulation work is given later in the article). Experimental testing may only be required for part of the separation scheme. A considerable amount of judgement is necessary to decide when experimental testing is appropriate and what level of testing is needed. Often, especially for early work, adequate experiments can be conducted in a simple batch column. In other situations, a continuous column is needed. Later-stage work often requires equipment representing the entire process. A secondary decision is required regarding the scale of the equipment. The "scale" is generally thought of as laboratory-scale equipment or a pilot-scale facility, but "lab-scale" and "pilot-scale" can cover a wide range of sizes, which might overlap.

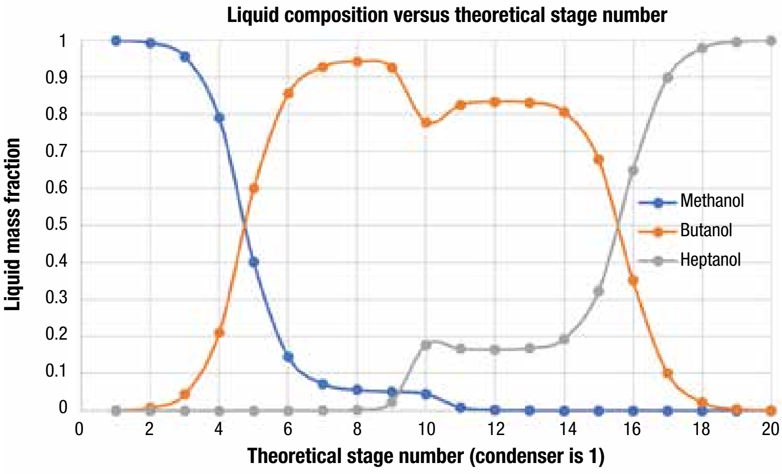


FIGURE 1. Relatively small amounts of intermediate-boiling compounds can build up to large concentrations within a distillation column, interfering with an otherwise easy separation. Feed to stage 10 is 1.0 kg/h of 50/50 methanol-heptanol. Feed to reboiler (stage 20) is 1.0 g/h butanol. Pressure is 760 mm Hg and the reflux ratio is 2

Concepts for experimental validation

In any attempt to compare experimental distillation results to simulation predictions, there are three main concepts that interact to influ-

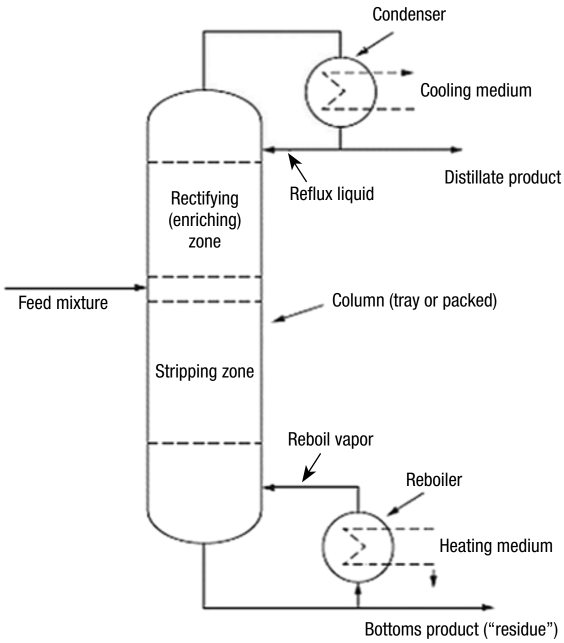


FIGURE 2. Shown here is a schematic diagram of a conventional distillation column with a feed, and distillation and bottoms products

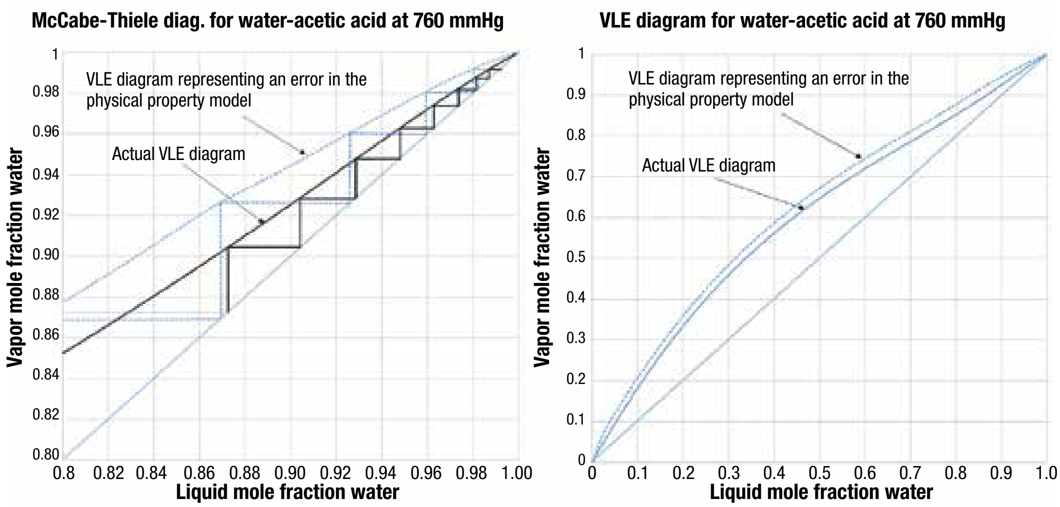


FIGURE 3. A positive error in the predicted VLE curve of a pinched binary system can cause the required number of stages to be significantly underestimated (The graph at the right is an expanded view of graph at the left)

ence the comparison. These are as follows:

- VLE of the components (and possibly LLE)
- Relative liquid-to-vapor flowrates (L/V ratios within the column)
- Vapor-liquid contactor efficiency (tray efficiency or packing height equivalent to the theoretical plate, or HETP)

When a disagreement exists between experimental distillation data and the corresponding simulation results, it will likely be a difficult challenge to determine which one, or more, of these effects are responsible for the discrepancy. Some additional detail is justified to explain their interaction.

For the sake of simplicity, the following discussion will refer to a binary system of components and a conventional continuous column with an overhead distillate, a bottoms product, and a feed that is introduced somewhere within the column, as is shown in Figure 2. Although real systems are seldom binary, the relevant concepts are more readily explained using binary components. These same concepts will apply to multicomponent systems in a similar, but more complex form. Likewise, ideas presented using a conventional continuous column can be extrapolated to more complex columns with multiple feeds, sidestreams and so on.

Vapor-liquid equilibrium. The relative volatility of an ideal binary chemical system is equal to the ratio of the pure component vapor pressures. If the components' interactions are not far from ideal and the two components have sufficient relative volatility (>2), then small errors in the VLE predictions may not significantly affect the separation. However, if the relative volatility is small (<1.5), any deviations between predicted and actual VLE will lead to large differences between the actual and predicted number of stages required to accomplish the desired separation.

Non-ideal systems will often have a pinch at the upper or lower end of the binary VLE curve. The term "pinch" means that the vapor and liquid compositions of the light-boiling component are nearly equal (this concept also applies to the heavy-boiling compound). The pinch is usually at the upper (right-hand) end of the VLE curve, which is the case for

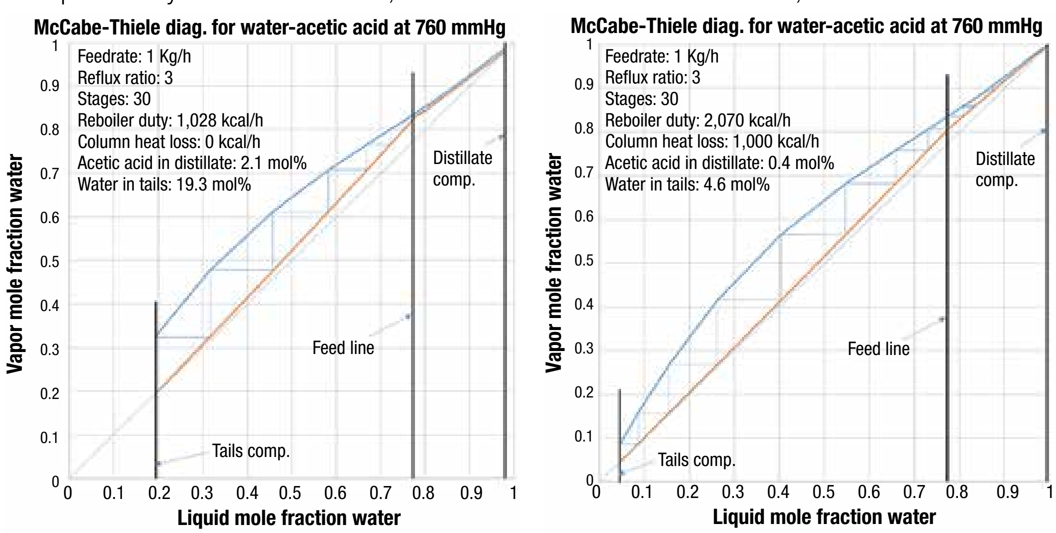


FIGURE 4. The left figure represents a column with no heat loss, whereas in the right figure, 50% of heat from reboiler is lost through the column walls. Laboratory columns with many trays at high temperature could easily have 50% heat loss or greater. The increased internal reflux improves separation, but also increases reboiler duty and reduces column capacity

binary pairs that repel each other. In this situation, the actual vapor pressure of the heavy-boiling component is nearly equal to that of the light-boiling component, due to the increased liquid-phase activity coefficient of the heavy-boiling component at infinite dilution. With sufficient non-ideality, the activity coefficient of the heavy-boiling component will become even greater, causing the heavy-boiling component's actual vapor pressure to exceed that of the light-boiling component at infinite dilution of the heavy-boiling component. This is the case for minimum-boiling azeotropes, and at the azeotrope composition, the actual mixture vapor pressures (pure component vapor pressure times activity coefficient at the component's liquid concentration) of the two components will be equal.

The closer the composition is to a pinch zone or azeotrope, the greater will be the effect of any errors in the prediction of the VLE on the separation. Figure 3 shows how a positive error in the VLE diagram can result in a significant underestimation of the number of stages required. Also, near a pinch or azeotrope, small changes in the reflux ratio can cause significant changes in the separation. A small error in the VLE prediction by the simulator could have a similar effect to a small change in the reflux ratio. It may be difficult to determine which is causing any discrepancies between a simulation prediction and the experimental results. If the components are so non-ideal as to cause phase separation within the column, then accurate LLE predictions will be necessary to produce accurate VLE predictions.

Liquid/vapor ratios. The relative vapor-to-liquid flowrates within the column are not only determined by the feedrate, reflux ratio, boilup ratio, and distillate-to-bottoms ratio, but also by heat effects. Excessive heat loss from a high-temperature column with many stages can significantly increase the internal reflux. This heat loss reduces both the liquid and vapor flowrates as one progresses up the column. The L/V ratio will be the lowest at the top of the column, where it can be experimentally determined from the reflux and distillate flowrates. However, the L/V ratio will progressively increase as one moves down the column, due to condensation of

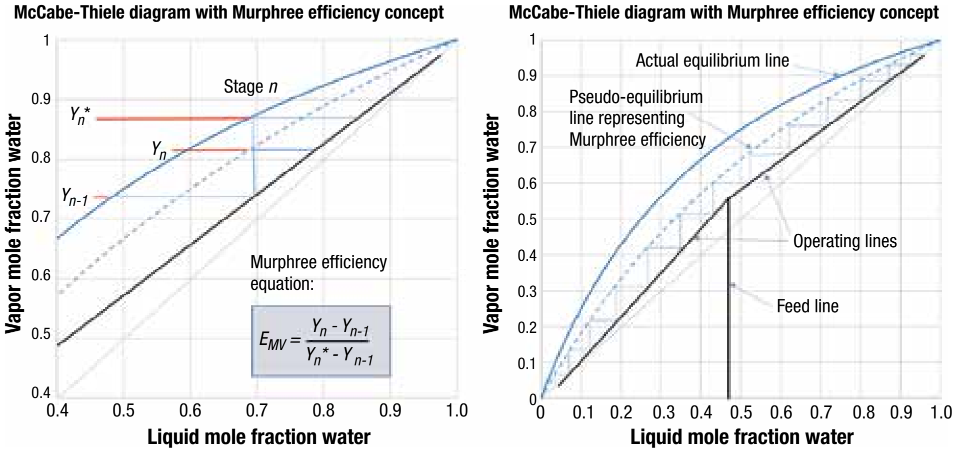


FIGURE 5. The Murphree vapor efficiency represents how close the actual vapor composition comes to reaching equilibrium with the liquid on an actual distillation tray. The concept of the non-attainment of equilibrium can be represented as a pseudo-equilibrium line on a McCabe-Thiele diagram, in which actual trays are drawn instead of theoretical trays [*5*]

the vapor. This effect can be thought of as an increase in the effective reflux ratio going down the column. This increase in L/V ratios due to heat loss will cause the column to have a better separation than predicted by a computer simulation, but at the expense of higher energy costs and lower capacity than expected (see Figure 4). Without understanding that the actual L/V ratios are different than expected, the VLE curve would appear to be more open (higher relative volatility or less pinched) than is actually the case. Preheated feeds and reflux from the condenser that have heat qualities different than expected can have similar effects on the column internal flows. Sub-cooled feed or reflux will cause condensation, which increases the L/V ratio below its point of entry into the column. Superheated or flashing feed may produce vapor flowrates different than anticipated, affecting the L/V ratio above the feed point.

Efficiencies. Process simulators generally use theoretical stages to represent the trays in a distillation column. However, in real columns, the vapor leaving a tray is seldom in equilibrium with the liquid from that tray. The difference between the actual and equilibrium vapor compositions can be expressed as an efficiency. A common method of defining efficiencies for actual distillation trays is the Murphree vapor efficiency (see Figure 5). Values for Murphree vapor efficiency tend to be in the range of 50 to 75% for laboratory- and pilot-scale columns, but can lie outside of this range. The Murphree vapor efficiency is an indication of how closely the vapor composition in an actual distillation tray approaches equilibrium with the liquid leaving that tray, as shown in the left-hand diagram of Figure 5. For a binary chemical mixture, if the vapor composition for every actual tray were plotted against the liquid composition on that tray, it would appear as a pseudo-equilibrium curve, as shown in the right diagram of Figure 5. The McCabe-Thiele concept could be applied to this pseudo-equilibrium curve, in which actual trays would be drawn, instead of theoretical stages, as for a true equilibrium curve.

If the Murphree vapor efficiencies for the trays of a distillation column are 100%, the number of actual trays required to accomplish a separation would be equal to the number of theoretical trays required. When the Murphree vapor efficiencies are less than 100%, the required number of actual trays will be greater than this theoretical number. Therefore, if the actual tray efficiencies are less than predicted, more actual trays will be required to accomplish a desired separation than would be anticipated based on the required number of theoretical trays and the predicted efficiency. Without properly accounting for the reduced efficiency, the separation will appear to be more difficult than predicted.

The efficiency of packed columns is routinely expressed as HETP (height equivalent to a theoretical plate). If the actual HETP is greater than predicted (less efficient), the column will contain less theoretical stages than predicted and this will produce similar results to a column with trays that have reduced efficiencies.

The tray efficiency is dependent on several factors, including the configuration of the tray (hole size, number of holes, hole area) or packing (surface area, shape, void fraction), the properties of the chemical mixture, the liquid and vapor flowrates, the L/V ratios, and the pressure. Several authors provide methods for estimating tray efficiencies [*1–4*].

Effect of pressure on the separation. The previous discussion shows how the VLE, L/V ratio, and contactor efficiency are intertwined, and the importance of knowing the values of each of these for the experimental validation of distillation columns. Another variable that needs to be considered is pressure. Pressure

not only affects the temperature, but can also change the VLE curve, as shown in Figure 6. Lower pressure often makes the VLE curve more open and the separation becomes easier at lower pressures.

Trayed plant columns usually have significantly higher pressure drops than laboratory or pilot columns. Therefore, if a laboratory or pilot column is used to validate simulation results, and it is operated at the same head pressure as that intended for the plant column, the laboratory or pilot column will have a lower base pressure than the corresponding plant column. For columns operating in the range from moderate vacuum to above atmospheric pressure, the effect on temperature and separation may not be significant. However, for high-vacuum columns with many trays, a laboratory or pilot column may have a much lower base pressure than the commercial column and a correspondingly lower base temperature. Generally, this lower pressure in the experimental column allows easier separation properties than the corresponding plant column.

In addition to overestimating the separation capabilities of the plant column, the laboratory or pilot column may underestimate the amount of degradation that will occur in the base of the plant column, since the plant column's base pressure and temperature will be higher than for the laboratory or pilot column. To overcome these problems, it may be necessary to operate the small-scale column at the same base pressure as intended for the plant column, or to run separate experiments, matching the head pressure in one test and the base pressure in another.

A case study

An example of how simulation discrepancies can be resolved using batch distillation experiments is presented here.

A client was interested in developing a method to continuously separate a mixture of ethylene glycol (EG), propylene glycol (PG) and 1,2 butanediol (1,2 BDO) in water. Distillation was one of the options being considered for the continuous commercial separation. The components had similar boiling points and the desired purity could not be achieved under modest positive pressures. From past experimental knowledge and experience, a subject-matter expert (SME) was aware of how this separation would take place under vacuum, and the simulation work progressed to consider vacuum separations. Initial simulation studies evaluated the separation of a known composition of the mixture using a combination of columns. Different physical property models, including NRTL (non-random two-liquid), UNIQUAC and Wilson, were tried based on the expected interaction of the components. The interaction parameters were estimated for the expected range of conditions for each model. However, the simulation results did not always demonstrate the expected separation. The results did not appear correct and often were very different from one physical property model to another.

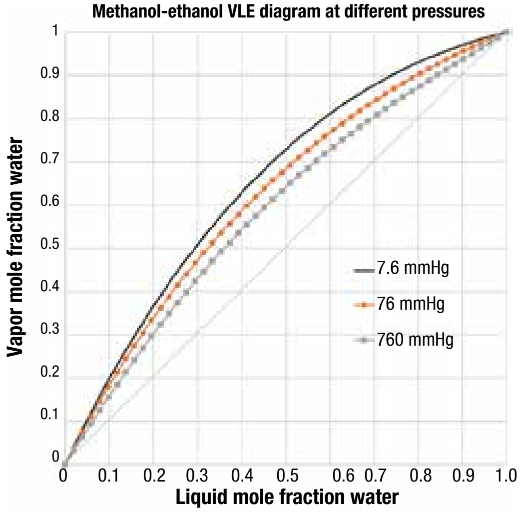


FIGURE 6. For the methanol-ethanol binary system, lower pressure opens up the VLE curve, which would make a distillation separation less difficult

A simple batch distillation experiment was set up to perform a validation experiment to confirm that the separation could be accomplished. The apparatus used was a 1-in. glass Oldershaw column with an evacuated and silvered jacket. Fiberglass insulation was added around the column and around the top of the glass kettle. The starting mixture of the chemicals was heated in the base and the column was operated in total reflux until it reached steady state. After that, the reflux ratio was changed and a total of ten distillate samples were collected.

A software package called Aspen Batch Modeler was used to simulate the unsteady-state batch distillation. The software simulates the batch distillation process dynamically, allowing the user to specify changing experimental conditions, including reflux ratios, distillate collection and so on. This software accesses the same Aspen properties library as Aspen Plus, which was being used to simulate the commercial distillation columns. Thus, once the optimum physical property model and parameters were found that allowed the batch simulation to match the batch experimental data, this model and the corresponding parameters could be used directly in Aspen Plus to simulate the commercial continuous case.

The mass of the components in the overhead distillate samples in the batch ex-

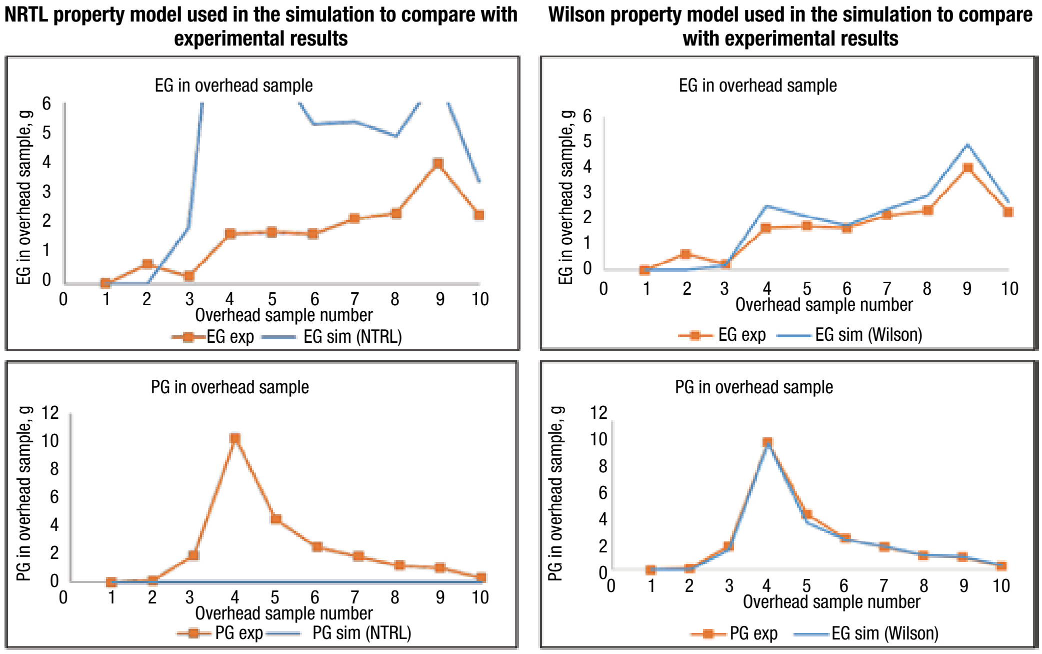


FIGURE 7. The Wilson property model provides a much better fit than the NRTL model. The above figures show the results for the mass of ethylene glycol (EG) and propylene glycol (PG) collected in the overhead sample in the experiment as compared to the simulation. The figures on the left compare the experimental data with the simulation when using the NRTL property model, while those on the right show a comparison when using the Wilson property model. The binary parameters were estimated using UNIFAC for both cases

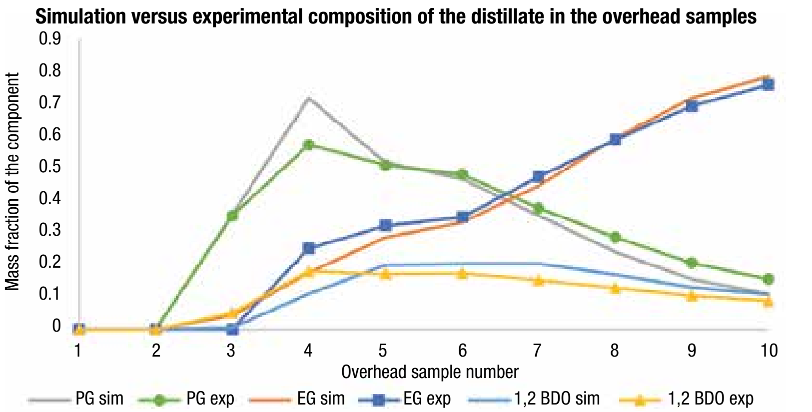
periment were compared to the simulation. Because of the expected component interactions, activity coefficient models were used. Specifically, the NRTL, UNIQUAC and Wilson property models were individually evaluated. For each of these models, different parameter estimation techniques were tried. Binary parameters were calculated by regressing data from the literature. The Antoine's parameters were calculated from literature data at the conditions of interest. Also, UNIFAC was used to estimate the binary parameters at the operating conditions. The best match to the experimental data was obtained using the Wilson property model. Figure 7 shows the close fit of the simulation results using the Wilson model and the contrasting poor fit when using the NRTL model.

The results for the NRTL case showed only EG and water (not shown in the Figure 7) being recovered in the distillate. No PG recovery was seen in the simulation in contrast to the experimental data. The results of the Wilson case, however, compared much better with the experimental results. Using the Wilson property model and optimized parameters, the results for the mass fraction of EG, PG and 1,2 BDO are compared with the experimental data in Figure 8. The data show a very good fit. The quality of this fit demonstrates that the Wilson property model corresponding parameters are appropriate for the subject conditions, and that they can be used with confidence in the simulation of the continuous commercial columns.

The commercial distillation column simulations in Aspen Plus were then re-developed utilizing the Wilson model and the data from the experimental batch distillation. The revised simulations showed distillation to be a feasible separation technology, including from a capital and operational cost perspective. Later, a client SME validated the distillation column simulation results based on experience in an existing plant with similar separations.

In this case study, the batch distillation experiment was useful not only to validate the feasibility of the separations, but it also provided data to calibrate the simulation model and to thereby add confidence to the commercial predictions.

FIGURE 8. Mass fractions of the components in the distillate overhead samples are compared with the optimized batch column simulation results when the using the Wilson property model. A very good match was obtained using the Wilson property model



Concluding remarks

The use of process simulation tools for modeling distillation columns is invaluable for designing plant-scale columns. However, it can be difficult to know if the simulator is generating accurate predictions. Additionally, there are potential problems associated with distillation columns that process simulators

do not address. Hence, experimental distillation studies are quite important to either verify the simulation results or to provide a path forward to improve the simulations. In this article, a case study was presented of a simulation effort that yielded some uncertainties, which were then readily resolved with laboratory batch-column testing.

When contemplating the need to experimentally validate distillation simulations, key points include the following:

- For process simulations, developing the proper physical property model by selecting the correct pure component properties, thermodynamic equations and component interaction parameters can be a challenging task, especially for moderate to severe non-ideal mixtures.
- Without experimental validation, it is difficult to know if the simulations are accurate
- Byproduct generation, foaming and fouling are difficult or impossible to predict by process simulators.
- Experiments should be conducted to validate distillation simulations and to determine if other non-simulated problems will occur.
- The main concepts that affect the separation in a distillation column are the VLE, L/V ratios, and contactor efficiencies (pressure also plays a role).
- When a disagreement exists between experimental distillation data and the corresponding simulation results, it will likely be a difficult challenge to determine which one, or more, of these effects are responsible for the discrepancy. ■

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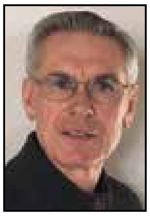

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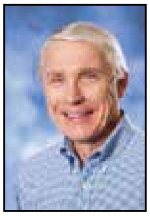

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Distillation, Part 2
Bubble-Cap Tray Vapor Turndown

The concept of tray stability can apply to bubble caps and be used as an alternative method to determine the minimum efficient capacity of these devices. A new stability correlation for bubble-cap trays is proposed and checked against FRI data

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Sulzer Chemtech USA, Inc.

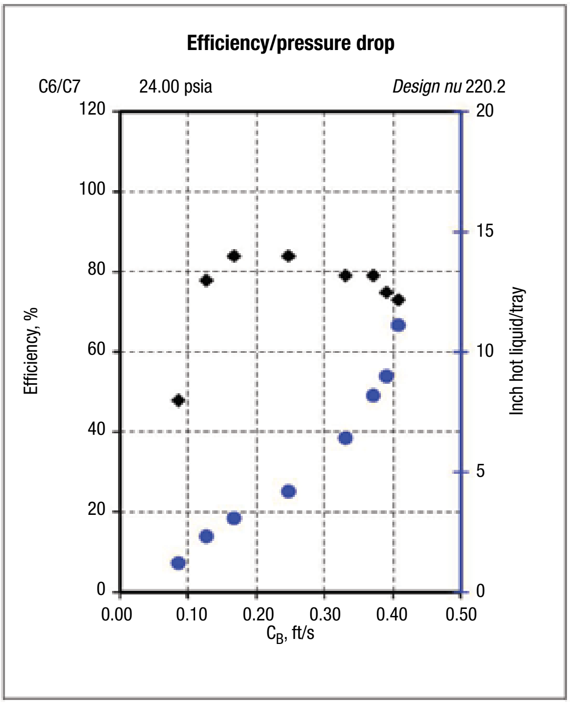

FIGURE 1. This graph shows typical bubble-cap operation at a pressure of 24 psia

The bubble-cap tray has been in the market place as a distillation device since the early 1800s [*1*]. It has been used extensively on distillation tray equipment worldwide as a highly efficient vapor/liquid-contacting device. Many people have examined the maximum capacity of bubble caps [*2, 3*], but very few have studied turndown. A U.S. Patent from 1987 [*4*] endeavored to enhance the turndown capability of bubble-cap trays to as high a turndown ratio value of 15:1. It is the intent of this article to establish a turndown criterion for bubble-cap trays such that the tray designer can maintain efficient operation at the lowest loads. A relationship is established, based on operational data, that shows what the minimum efficient vapor load can be on bubble-cap trays.

Bubble-cap tray and turndown

The stability of sieve trays, movable-valve trays and fixed-valve trays was discussed in Ref. 5. The theory presented there is that there is a relationship between the upward force of the vapor to a tray that will balance against the gravitational force of the liquid (froth) depth and maintain good efficient vapor distribution onto the tray. Maintaining good vapor distribution should enable good tray performance. A "stability" term was introduced that was basically a modified Froude number. Bubble-cap trays were excluded from the discussion at that time because the liquid is not balanced against the vapor on such trays. The liquid is prevented from weeping through a bubble-cap tray by the physical presence of the bubble cap risers.

However, questions have arisen about the turndown capability of bubble-cap trays. Normally the topic of turndown is not an issue, since trays that have a loss of efficiency (and theoretical stages) at turndown can easily be compensated by an increase in reflux ratio (heat duty) to the tower. How-

ever, there are times (in highly heat-integrated units) when there is little or no extra heat available to overdrive the tower when operated at turndown. In these cases, the issue of efficient turndown of bubble cap trays becomes extremely important.

With the typical sieve or valve tray, the prevalence of weeping can be one way to determine the minimum operating vapor load to such a device. As mentioned above, the author has offered an alternate idea to weeping on how to determine the turndown of such typical trays with the introduction of the "stability" concept:

$$\eta = (\Delta P_{DRY}/H_S)^{0.5} \quad (1)$$

Where:
η = stability factor
ΔP_{DRY} = inches of liquid
H_S = Hydrostatic head of liquid on the tray, inches of liquid

This stability concept should, in theory, be applicable to bubble-cap trays with some modification. The theory is that to maintain good efficient operation of a bubble cap tray, the vapor must be flowing through a high percentage of the bubble cap's risers.

One modification to the concept of Equation (1) would be that the hydrostatic head of liquid has to have the height of the slots on the bubble caps removed. The vapor that is introduced to the liquid on a bubble cap tray does not have to "fight" against the full depth of liquid (or froth) on the tray to be able to flow through the cap. The other modification to Equation (1) is the definition of dry tray pressure drop itself. Dry tray pressure drop is a simple theory that has been explored by the author in other articles [6–8].

$$\Delta P_{DRY} = 12\rho_v(V_H/C_V)^2/2g_c\rho_L \quad (2)$$

Where:
ΔP_{DRY} = inches of liquid
V_H = Hole velocity, ft/s
ρ_V = Vapor density, lb/ft^3
C_V = Orifice coefficient
ρ_L = Water density, lb/ft^3
g_C = Acceleration of gravity = 32.174 ft/s^2

If one assumes that the four critical areas of a bubble cap are equal (riser area, reverse area, annular area and slot area) or are at least limited by the riser area, then the dry-tray pressure drop through the riser can be used to establish the ΔP_{DRY} in Equation (2) above. The C_V for smooth-bore risers can be assumed to be 0.43. With this, Equation (2) reduces to the following:

$$\Delta P_{DRY} = 1.009(\rho_V/\rho_L)V_R^2 \quad (3)$$

Where:
V_R = Riser velocity, ft/s

The data to test the validity of this theory were established by Fractionation Research Inc. (FRI) in Alhambra, California between the years 1956 and 1968 [9]. The data were taken in an industrial-size tower (48-in. dia.) at total reflux and show the tray efficiency versus vapor load. There were 125 data sets taken during this time period with numerous compounds operating from deep vacuum to 500 psia. Figure 1 shows an example of one such data set with cyclohexane/*n*-heptane

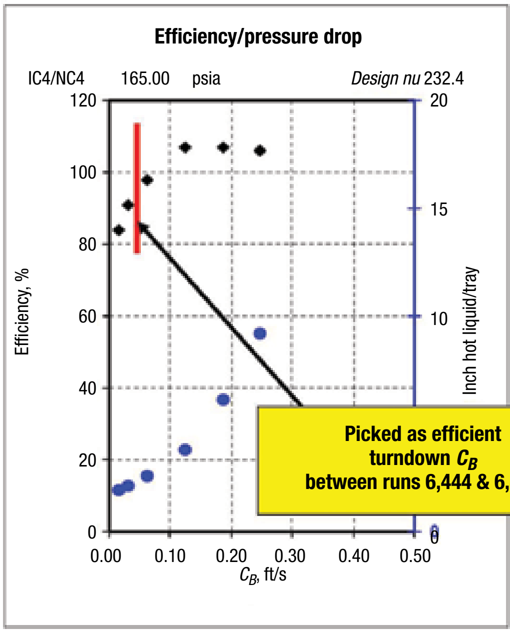

FIGURE 2. This graph was used for determining the turndown of the C-factor, C_B

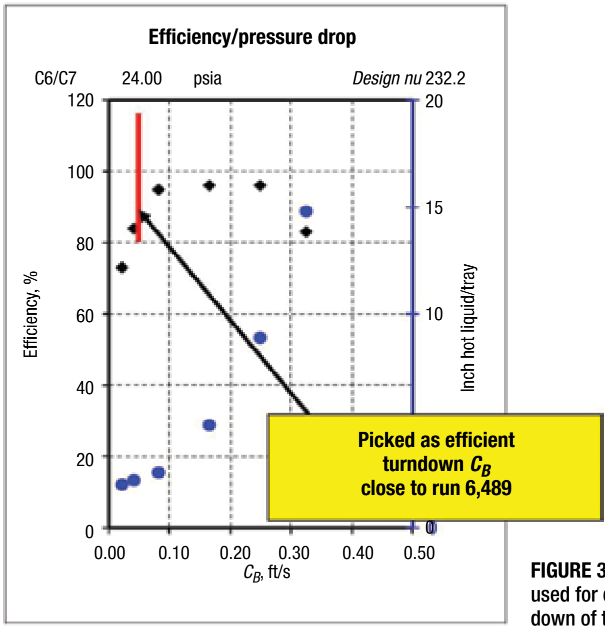

FIGURE 3. This graph was used for determining the turndown of the C-factor, C_B

TABLE 1. DATA FROM TWO POINTS IN FIGURE 2 AT TURNDOWN									
Run	Riser area, ft^2	Vapor density, lb/ft^3	Liquid density, lb/ft^3	V-rate, lb/h	CFS	Vr, ft/s	Dry drop, in. of liquid	H_S, in. of liquid	Stability
6,444	1.3906	1.74	30.7	14,720	2.3499	0.1690	0.1633	2.34	0.2641
6,445	1.3906	1.74	30.7	7,370	1.1766	0.8461	0.0492	2.06	0.1409

TABLE 2. DATA FROM TWO POINTS IN FIGURE 3 AT TURNDOWN									
Run	Riser area, ft^2	Vapor density, lb/ft^3	Liquid density, lb/ft^3	V-rate, lb/h	CFS	Vr, ft/s	Dry drop,	H_S, in. of liquid	Stability
6,488	1.3906	0.305	42.7	9,850	8.9709	6.4513	0.2998	1.99	0.3882
6,489	1.3906	0.302	42.5	4,940	4.5438	3.2676	0.0765	2.02	0.1946

operating at 24 psia pressure. One can see that where the tray efficiency drops from about 80% to less than 50% as the C_B falls below 0.1 ft/s, that this would be an indication of minimum efficient operation. (Note: The C-Factor, C_B, is a vapor load factor based on the bubbling area.).

A review of the available data was carried out to determine suitable cases to validate the theory. The data sets from FRI included an indication of weeping from the trays. Normally a bubble-cap tray should not weep, because most trays are either welded in or fully gasketed. The FRI trays were neither, since operators have to change out the trays frequently to be able to test more trays quickly. The weeping observed was present at the tray seams and at the tray support rings in the FRI column. Recent work at FRI has shown that even minor wall weeping or leakage can cause a significant loss of tray efficiency at low vapor rates. Due to this, data exhibiting signs of weeping were excluded.

Most of the tray data were for bubble caps 4 in. in size. Of the 4-in. caps reported, there were two styles; slotted and “tea cup.” There was a comprehensive set of data from the “tea cup”-style caps that covered a wide set of pressures. In addition, by examining data from the “tea cup” cap, which is the industry standard today, all subjectivity with regards to slot shape and size is eliminated from the discussion.

TABLE 3. TEA-CUP BUBBLE-CAP STABILITY			
System	Pressure, psia	Run numbers	Stability
i/n C4	500	8,307–8,313	0.19
i/n C4	400	8,297–8,303	0.18
i/n C4	300	8,280–8,286	0.20
i/n C4	165	6,441–6,446	0.20
C6/C7	24	6,485–6,490	0.20
C6/C7	5	6,517–6,520	0.21

Examination of the data did lead to some subjectivities. Namely, what is a tolerable reduction in tray efficiency at turndown? Figure 2 shows what was picked as the turndown limit of efficient operation (which was about a 10% loss in tray efficiency) for a set of data at 165 psia. The tray geometry examined here is reported thoroughly in Ref. 9. The inner diameter is 47.75 in., distance to outlet weir from tray centerline is 15 in. and the flow-path length is 30 in. The outlet weir height is 2 in. There are 37 bubble caps per tray, each being 4 in. in size and having a 1⁄4-in. gap under the cap. The downcomers are sloped, and there is a recessed inlet pan. The outlet weir length is 37 in. Table 1 shows the examination of the two data points surrounding this choice of minimum tolerable operation in Figure 2. The value of the stability between these two data points is about 0.2.

The exact same trays were also operated in C6/C7 service at 24 psia (Figure 3). Here the 10% loss of efficiency is very close to the data point at run number 6,489. Table 2 shows the examination of the two data points surrounding this choice of minimum tolerable operation in Figure 3. The value of the stability between these two data points, and close to run 6,489, is about 0.2.

Repeating this procedure for all the other “tea cup” data sets yields an interesting set of results, as shown in Table 3. It appears that there is a constant stability factor number for turndown of 4-in. “tea cup” bubble-cap trays. This value is approximately 0.2, which is considerably smaller than other trays as reported earlier. Ref. 5 shows that most other trays need to stay above a stability number of 0.6 to remain efficient. It makes sense that bubble-cap trays can use a smaller stability number since they should not weep.

TABLE 4. DATA FROM TWO DATA POINTS IN FIGURE 4 AT TURNDOWN									
Run	Riser area, ft^2	Vapor density, lb/ft^3	Liquid density, lb/ft^3	V-rate, lb/h	CFS	Vr, ft/s	Dry drop,	H_S, in. of liquid	Stability
4,100	1.1873	0.31	41.9	9,080	8.1362	6.8527	0.3504	5.38	0.2552
4,101	1.1873	1.31	41.9	4,600	4.1219	3.4716	0.0899	5.65	0.1262

Keep in mind that all tray data examined thus far used only a 2-in.-high outlet weir. The question remains, "What happens when a different outlet-weir height is chosen?" There was one set of data examined at FRI using very tall 6-in.-high outlet weirs. The bubble caps for this data set were slotted, not "tea cup." This data set (runs number 4,094–4,101 operating at 24 psia) was thus examined to see if a stability of 0.2 was reasonable for this unusually tall outlet-weir height.

Figure 4 shows this data set and Table 4 shows the examination of the two data points surrounding the choice of minimum tolerable operation. Table 4 results did employ a reduction of the hydrostatic head due to the elevation of the 1.75-in.-tall slots on the bubble caps. The value of the stability between these two data points is again very close to 0.2. Therefore, a conclusion can be drawn that bubble cap trays can employ a minimum stability factor of 0.2 and that the correlation above can apply to both "tea cup" and slotted caps.

Summary

The concept of tray stability can be applied to bubble caps and can be used to predict the minimum efficient capacity of these devices. A new stability correlation for bubble cap trays has been developed and checked against FRI data. Based on this limited set of data it may be concluded that the tray stability correlation result needs to remain above a value of 0.2 for bubble cap trays. ■

Edited by Gerald Ondrey

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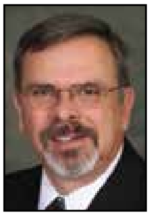

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For more on distillation, see Part 1, "Experimental Validation of Column Simulations," on pp. 30–37, and other articles in the *Chemical Engineering* archives at www.chemengonline.com.

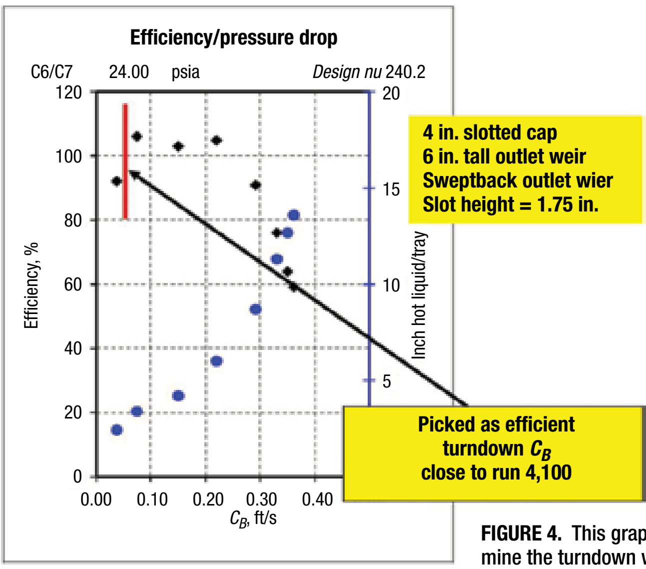

FIGURE 4. This graph was used to determine the turndown with a 6-in. outlet weir

Single-Use Gloves: Problems and Solutions

When wearing single-use protective gloves, sweat can create health and safety issues. Presented here is a look at the causes of the problems and possible solutions

Thomas Draskovics
SW Safety Solutions

IN BRIEF

A great many situations across the chemical process industries (CPI) require quality hand protection, both for worker safety and to prevent product damage or contamination. Examples include working with hygienic processes in the pharmaceutical industry, conducting laboratory research, taking and processing test samples, blending and compounding materials, working with paint materials and others. But regardless of the activity, the natural reaction of human hands to the tight, hot environment inside gloves is sweating. This natural skin response can make wearing gloves uncomfortable and lead to safety risks, as well as lead to skin problems that make the issue worse. Gloves are a necessary precaution, but without taking steps to reduce sweat buildup, gloves quickly become a source of discomfort and health issues (Figure 1). This article presents information about how problems related to sweat in single-use gloves are caused and offers some ideas on how to avoid them.

FIGURE 1. Single-use gloves protect hands, but also create an occlusive environment that can negatively impact hand health and job performance

Gloves and moisture

The tight, hot environment inside single-use (SU) gloves is a major cause of sweat and irritation for users in every industry. Moisture is one of the most common skin irritants in a glove-protected environment, especially when that moisture stays on the skin for long periods of time. When skin is exposed to sweat for a prolonged time, it weakens and becomes more vulnerable, and the moist environment is the perfect breeding ground for

bacteria and fungus. Wetness inside a single-use glove hinders users' ability to perform certain job functions by limiting dexterity, tactility and mobility. It can also become a safety hazard, since some workers will forego gloves altogether, rather than deal with the sticky, oppressive feeling of a wet glove [*1*].

Standard single-use gloves provide a non-permeable barrier that protects workers' hands in light-duty work environments. However, they also create a highly undesirable result — a harsh, occlusive environment between the glove and hand that can negatively impact hand health and, ultimately, job performance. Lack of airflow inside the gloved hand inhibits its proper regulation of the skin environment, glove friction from repeatedly rubbing against the skin harms the upper skin layers, and higher temperatures within the glove increase perspiration and discomfort. Additionally, this occlusive environment serves as a breeding ground for bacteria, fungus and other nasty elements that can negatively impact hand health in many ways, especially given that the skin on human hands is much thinner than on other parts of the body.

Imagine wearing a single-use glove in the workplace for hours at a time over a period of days, months and even years. Add in the fact that your hands are "working hard" inside the glove while you grip, move, rub and so on, to complete your work tasks. This leads to friction and mechanical abrasion of the skin further exacerbating an already difficult hand environment. Hand skin layers can become macerated, reducing the skin's ability to react defensively to external substances, and exposing the skin to even more serious afflictions.

Skin biology

From a physical perspective, where the hand first comes in contact with the occlusive environment, the acid mantle is disrupted and the stratum corneum — the outer most layer of the skin — can become compromised. The outermost section of skin (stratus corneum) has three layers itself. The innermost layer is the actual barrier that regulates absorption into the body. The outermost layer contains cells that, although are not dead cells, have no development process left — they merely serve as the frontline in regulating moisture within the body and keeping unwanted elements out. The middle layer exhibits properties of both the outer and inner sections, a kind of mixing of the two functions.

As the occlusive environment persists, deeper damage begins to take place with the skin structure. Proteins and lipids are stripped away, so skin is unable to keep its natural moisture intact. Barrier protection begins to break down. While sweat contains small amounts of salt and miniscule levels of other waste products, it is predominantly water, and that is what causes most of the damage from prolonged exposure. It can take as little as 72 hours of exposure to water, whether in sweat or elsewhere, to cause significant skin damage [*2*]. With an occlusive glove environment wrapped around the hands during an eight-hour workday, skin health can be impaired to the point of injury in less than two weeks.

Skin pH is slightly acidic, ranging from 4.0 to 6.5 in a normal environment. Inside an SU glove, your hand loses moisture (sweats) and pH levels quickly rise, further affecting the skin surface and underlying layers. The skin's ability to regulate its surface diminishes, and the resulting alkaline environment can actually accelerate bacterial growth. The longer the glove remains on your hand, the more damaging this occlusive environment becomes, increasing the likelihood of skin dryness, redness and irritation.

Over time, health risks for workers from uncomfortable SU gloves can greatly decrease productivity, encourage more frequent workplace safety violations and increase the risk of significant medical issues, all of which lead to much higher costs for employers. By limiting hand functionality, perspiration may hinder a worker's ability to perform certain job functions, or cause them to change gloves more frequently. Yet, repeatedly alternating from a wet to dry environment, like donning and removing several pairs of gloves a

day, exacerbates skin irritation. Some workers may forego wearing protection entirely rather than endure the clammy, suffocating feeling of a wet glove, dramatically increasing the risk of safety issues and the potential for worker injuries. According to the U.S. Centers for Disease Control and Prevention, about 70% of workers who experience hand injuries were not wearing gloves at the time [3].

FIGURE 2. Glove changes and lotions can present their own issues

Contact dermatitis

In its normal state, the skin has a low permeability rate, but as barrier function is compromised, that rate begins to increase, exposing the skin to more irritants. The prolonged moisture, increased temperature and unbalanced pH level provide more opportunities for bacteria and other external contaminants to enter the skin, causing further irritation.

Both occlusion and fluctuations in environment with an SU glove can cause a host of skin conditions, such as redness, dryness and chapping. If skin has been repeatedly damaged or these conditions are accelerated by an allergic reaction, bacteria and other unwanted external elements more easily pass through the skin's compromised barrier. Left untreated, this volatile combination causes increases in skin irritation that can lead to more serious conditions, such as chronic contact dermatitis, one of the most commonly reported occupational diseases. Occupation-related contact dermatitis, classified as either irritant or allergic, can develop from frequent and repeated use of hand-hygiene products, exposure to chemicals and SU glove use.

Irritant contact dermatitis in particular often stems from sweat management issues, and is a very common ailment of SU glove wearers. It is non-allergic, meaning the skin has not reacted with any contaminants or ingredients that served as the irritant. Rather, it stems from the skin coming in frequent contact with a harsh environment that produces dry, itchy, irritated areas around the points of contact, such as repeated hand washing or prolonged exposure to an occlusive environment.

By comparison, allergic contact dermatitis (type IV hypersensitivity) results from exposure to accelerators and other chemicals used in the manufacture of rubber gloves, as well as from exposure to other chemicals found in industrial settings. Allergic contact dermatitis often manifests as a rash beginning hours after contact and, like irritant dermatitis, is usually confined to the areas of contact. Latex allergies are one possible cause of allergic dermatitis, and as a result nitrile gloves have seen a growth in production from glove manufacturers compared to latex equivalents.

Nitrile is a synthetic rubber copolymer of acrylonitrile (ACN) and butadiene, and has been shown to be more resistant to certain oils and acids than natural rubber, while maintaining similar levels of comfort and flexibility to latex. However, some skin issues attributed to latex allergies are misdiagnosed, being rather caused by exposure to accelerators and other chemicals used in the manufacture of both latex and non-latex gloves, such as dithiocarbamates, thiurams, and mercaptobenzothiazoles. These mistaken allergies can be prevented by utilizing gloves that are thoroughly washed after manufacturing, as some glove producers offer to increase user comfort.

While irritant dermatitis is a much more pressing issue when it comes to sweat management, all forms of dermatitis can not only be detrimental to the health of the worker, but also extremely costly to the employer. OSHA (Occupational Health and Safety Administration) calculates that a single case of dermatitis can cost over $11,000 in employer-paid expenses [4].

Glove changes and skin lotions

Common moisture management techniques include frequent glove changes (Figure 2) to limit exposure to prolonged moisture, as well as emollients and creams that provide an additional layer of protection between glove moisture and the skin. Most lotions designed to promote skin healing will serve this end, in particular those containing petrolatum, oat or dimethicone, as they are likely backed by clinical trials [5].

But glove changes impede productivity, since you need to pause work to switch gloves. And as noted above, constantly alternating between environmental extremes can do more harm than good. There are no clear guidelines for how frequently one should switch gloves to prevent skin damage, considering most of the time glove changes are not enough to notably prevent injury if not paired with other solutions.

Likewise, in certain instances, the slippery layer of a cream could negatively impact dexterity and tactile sensation, leading to potential hazards and compromises in safety within the work environment. Skin care products must not undercut the efficacy of antimicrobial soaps and rubs, nor compromise the glove materials used in the working environment. Adding lotions or creams can complicate the overall compliance process, unnecessarily increase donning time and ultimately increase cost per use.

Newer technologies

Sweating while wearing a single-use glove is inevitable, but managing moisture is vital for worker health and productivity. Newer technologies within a glove help manage this interior environment and make the wearing experience much more comfortable and productive, while providing benefits that protect skin from the occlusive environment itself.

One such technology incorporates an absorbent liner that wicks moisture from the skin. SU gloves with an interior moisture-wicking layer help prevent irritation, as well as provide a safer environment for skin to heal if it has experienced any trauma that left the skin surface compromised. This layer is typically a cotton-based

powder or dust-like material, and is applied via a spray adhesive on the glove interior. In other words, creating a dryer ecosystem within the glove provides a healthier environment for the hand. By absorbing hand sweat as it is produced, users can prolong the use of one pair of gloves for hours, up to a full work day, without needing to change due to irritation. The structural integrity of the gloves is also extended, as interior moisture can cause latex or nitrile to weaken and eventually break. Additionally, therapeutic properties and protective ingredients manufactured right into a glove can limit the potential for irritation from the occlusive environment on the inside.

A common issue across industries is unreliable glove thickness. Some manufacturing processes produce gloves that vary significantly in thickness in different locations on the glove — during production, gravity can cause still-hardening latex or nitrile to pool at the glove cuff or fingertip, leaving some areas weak and prone to breaking or too thick and lacking in tactility. So some glove manufacturers have responded by employing additional techniques to ensure uniform glove thickness, resulting in gloves that are strong and tactile only where you need them to be.

Choosing the right glove — in terms of thickness, material, size and performance technologies — is essential, as these attributes all contribute to creating the ideal environment to promote proper hand health as well as optimum function. Exact user needs and corresponding glove characteristics, such as puncture or abrasion resistance, are mostly determined by application. Users need to consider whether there is time to change gloves or apply a sticky cream before donning gloves, or whether it is it best to use gloves that will provide a more balanced, safer hand health environment from the start. Workers and employers should also be sure to consider the occlusive environment and its effects before selecting the best gloves for their purposes. ■

Edited by Scott Jenkins

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Improvements in DP Level Measurement

Differential-pressure (DP) level measurements are widely used in chemical and petrochemical facilities, thanks to their reliability and ease of use. Recent advances are making them even more reliable and easy to use

Ehren Kiker
Endress+Hauser

Differential pressure (DP) level-measurement technology (Figure 1) is the most commonly used approach in the chemical process industries (CPI), thanks to its reliability, ease of use and adaptability to a variety of applications. While there are many benefits to working with DP measurement on level-measurement applications, there are some drawbacks, as well. Fortunately, several new advances in the design of seals and sensors, as well as new manufacturing techniques for filling remote-seal systems, are expanding the functionality of DP level systems into applications that previously required alternative level technologies. These advances are also improving the reliability of DP level measurement in existing applications and making it even easier to install.

FIGURE 1. Differential pressure is the most widely used level measurement method in the chemical and petrochemical industries

DP level measurement

DP level measurement has been used for decades, for many reasons. DP instruments are easy to install and configure, and the technology can be used in both open and closed tanks. The sensors do not have to be inside the tank, so internal obstructions are not a problem, and maintenance of the sensors does not require shutting down the process.

DP instruments can be used for a variety of measurement applications including level, flow, filter monitoring, measurement of gage pressure and more. Instrument technicians worldwide are familiar with the technology, so training is usually not required, and spare devices can be kept in stock onsite for use in many different applications.

DP instruments are adaptable to process conditions such as exposure to corrosive media, high or low temperatures, foaming, and clean or dirty fluids. For many reasons, DP has become the default technology for level measurement in many CPI facilities.

To measure level using DP, pressure from the high-pressure and low-pressure connections are sent to a DP transmitter (Figure 2). This is typically done via either impulse lines, or remote diaphragm seals with capillaries. Both types are commonly used in a variety of applications in the CPI and have different advantages and disadvantages.

An impulse line is a rigid metal tube that allows the process media to directly contact the DP sensor body. Impulse lines are easy to install onsite to a stock DP transmitter. They provide a fast response time to level changes, provide good accuracy for DP level measurements, and protect the transmitter from temperature extremes of fluids stored in the tank.

FIGURE 2. A DP level-measurement instrument consists of two pressure sensors — one above the maximum level and one at the bottom — and a transmitter that calculates level

But the fluid in the impulse lines can cause problems, mainly due to changes in viscosity as ambient temperatures change. This can cause inaccuracy in pressure readings, and hence level readings. If ambient temperatures become very cold, the fluid can freeze, leading to a total loss of measurement. Impulse lines can be insulated and heat-traced, but this adds costs up front and increases required maintenance.

On closed-tank applications, impulse lines use either a dry-leg or a wet-leg configuration. Dry- and wet-leg configurations are susceptible to measurement errors due to condensate collecting in dry legs, or evaporation causing loss of fluid in wet legs. Such applications require regular maintenance to ensure measurement reliability. Also, impulse lines are metal tubes, and can be difficult to fit into confined areas, particularly when insulated.

Remote diaphragm seals consist of a sensing diaphragm mounted on the side of the tank, and an oil-filled capillary tube connecting to the transmitter's pressure sensor. Unlike rigid impulse lines, the capillaries are flexible (Figure 3) and are hermetically sealed.

A variety of fill fluids are available to accommodate different process conditions, such as high or low temperatures, and the diaphragms are available in a wide range of materials to deal with corrosive process fluids. Remote seals can be provided with appropriate process connections and appropriate wetted materials to mount directly to a vessel.

But as with impulse lines, fill fluids are susceptible to temperature fluctuations, depending on the length and diameter of the capillary and the type of fill fluid. This can cause significant measurement errors. Remote seal systems typically have a slower response time compared to impulse lines. Larger diaphragms required for improved sensitivity and accuracy can result in higher costs, especially when exotic materials such as Hastelloy or tantalum, or larger flange ratings, are required.

Remote seal systems have higher stocking costs because they are all-welded systems. This reduces the flexibility of stocking items for several different applications, as can be done with impulse lines.

By using impulse lines and remote seal systems interchangeably — depending on the specific process conditions and requirements — users can employ DP level measurement in a wide variety of applications throughout a facility. The disadvantages of using impulse lines or remote seal systems lead to a small but not insignificant number of problems. Too often, these performance issues are tolerated due to a lack of an acceptable alternate level-measurement technology.

DP transmitters will provide extremely accurate and stable measurements across a wide variety of process conditions, but are dependent on sensors. New developments in both technology and production techniques are improving the sensing capability, so DP level measurement can be used in applications where either poor performance or high maintenance was previously tolerated. These advances include the following:

- Asymmetrical-flexing diaphragms for improved response time and reduced temperature effects
- Application-specific fill fluids to ensure improved

FIGURE 3. Remote diaphragm seals use flexible capillaries to send pressure to the DP transmitter

performance

- Electronic DP measurement for elimination of problems with impulse lines and remote seal systems

Different diaphragm types

Many issues that arise with DP measurements are related to remote seal issues, specifically temperature-related errors and response time.

Standard diaphragm seals flex symmetrically — that is, when pressure is applied, the diaphragm flexes the same in all directions around the center point. Diaphragm seals are designed to minimize the volume of fill fluid (to reduce process and ambient temperature effects) and the thickness of the diaphragm seal (to provide higher sensitivity). Seal manufacturers constantly strive to reduce the volume of fill fluid and diaphragm thickness to improve performance without compromising the integrity of the seal.

Symmetrically flexing diaphragms are susceptible to measurement errors and slower response times caused by changes in process and ambient temperatures.

Some manufacturers of diaphragm seal systems have recently started using seals that flex asymmetrically in opposite directions around the center point (Figure 4). The result is a diaphragm seal that flexes predictably with good repeatability, while using less fill fluid. This allows for thicker diaphragm seals that provide greater durability and maintain sensitivity for adequate turndown.

Some products have a seal profile that allows them to flex asymmetrically. The result is a diaphragm seal that has higher sensitivity and lower temperature-related measurement errors than symmetrical-flexing diaphragms (Figure 5).

Asymmetrical diaphragms can often provide improved accuracy and stability with smaller diaphragm seals compared to standard symmetrical-flexing diaphragms. As a result, the use of asymmetrical seals can allow designers to use smaller flange sizes for process connections. When dealing with large projects that require many DP level measurements — each needing high flange ratings or exotic materials — this option can result in significant cost savings. In addition, the ability to use a diaphragm with a smaller flange sizes can reduce costs due, by allowing for smaller isolation valves and other associated accessories.

Different filling options

Diaphragm seals are typically filled with a minimal amount of fill fluid to promote the best possible response time and sensitivity to pressure change. In standard filling processes, the seal itself is cleaned thoroughly and exposed to vacuum for a period of time, to get all the gas out before the filling is done. This is a critical part of the process because a small amount of residual gas in a diaphragm seal system can make a pressure measurement unstable

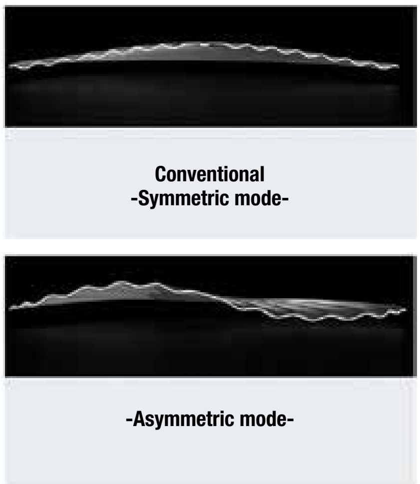

FIGURE 4. A symmetrical remote seal diaphragm flexes the same in all directions, while an asymmetrical diaphragm flexes in opposite directions

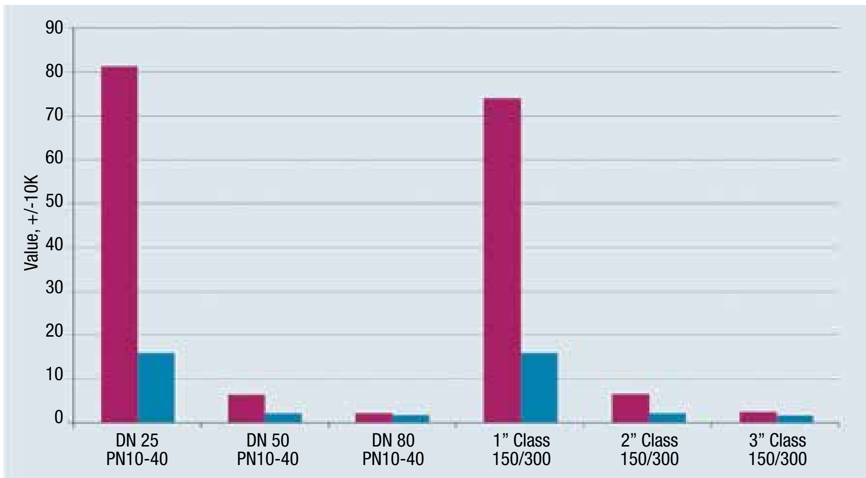

FIGURE 5. Temperature changes affect the accuracy of remote seal systems at various flange sizes. The red bars show errors with conventional symmetric diaphragm seals, while blue shows the lesser effect of temperature on asymmetrical remote seal diaphragms

FIGURE 6. Electronic DP level systems eliminate the need for impulse lines or capillary tubes because the sensors connect to the transmitter via wiring

and inaccurate.

Prior to filling, the fill fluid is treated to reduce its viscosity and ensure a good fill. Once the fill is completed and the capillary is welded to the transmitter, the pressure instrument is calibrated according to customer requirements.

This diaphragm seal-filling process is roughly the same in all filling facilities around the globe, regardless of supplier, but this "one size fits all" process does not account for the effects of application-specific process conditions, and these can adversely affect the measurement.

Recently, some manufacturers have begun using new filling methods to address this issue. In these new processes, the filling of the fluid under deep vacuum conditions is still more or less the same as standard procedures. However, the amount of fill fluid is now pre-determined per seal system. When the fill is performed, the amount of fill fluid that went into the diaphragm seal system is measured to ensure the device is filled completely.

The next step in this unique filling process is to determine the position of the measuring membrane. The position is adapted to the user's application, the type of fill fluid required, and material of the membrane itself. This means that if the customer provides process data that tell the manufacturer the seal will be exposed to a working temperature of 300°C (572°F), then the amount of oil and position of the membrane is corrected to ensure that the membrane is in its best possible position under those process conditions.

This new way of producing DP pressure instruments with diaphragm seals and capillaries gives users increased accuracy and more reliable process information under tough conditions.

Electronic DP level sensing

As mentioned previously, the major limitations when implementing a DP level-measurement system have nothing to do with the transmitter. Most problems instead arise with the impulse lines or remote seal and capillaries. Impulse lines are susceptible to plugging, leaking and icing — all of which negatively affect measurement. Remote seal systems are also prone to large measurement errors due to ambient and process temperature swings.

Until recently, the only solutions have been to use smaller-diameter impulse lines or capillaries — which adversely affect response time — or use costly insulation or heat tracing systems. Now many of those issues can be avoided by using electronic DP transmitters.

Rather than transmit pressure from the high-pressure and low-pressure connections via impulse lines or remote seal/capillaries, electronic DP transmitters measure level with two pressure sensors mounted at the top and bottom of the vessel. With this configuration, one sensor is always below the minimum process fluid level, and the other is always above the maximum process fluid level. Each sensor independently measures gage or absolute pressure, but sends signals back to a DP transmitter electronically. Sensors are mounted directly to the vessel, and signal wiring connects the sensors to the transmitter, thereby eliminating the need for impulse lines or capillaries (Figure 6).

Without the need for impulse lines or capillary tubes, an electronic DP transmitter eliminates issues related to leaking fittings, plugging, icing and slow response times. Advantages include reduced maintenance, minimal to no temperature effects, and fast and stable response times. An electronic DP system is modular, so components can be individually replaced as needed.

An electronic DP system can easily be retrofitted using the same process connections, mounting and wiring as the existing DP level system. The system connects to the same input point on the control system, with the same scaling as the DP level system being replaced.

With electronic DP level systems, end users can still have the advantages of DP level measurement, while eliminating many of the disadvantages limiting applications.

Closing thoughts

While there are many different level measurement technologies, DP is the most commonly used in chemical and petrochemical facilities. Conventional DP level measurement can be susceptible to a variety of issues, such as plugging of impulse lines or temperature-related drift when using remote seals and capillaries. Fortunately, manufacturers are developing new technologies, such as asymmetrically flexing diaphragms, application-specific filling techniques, and electronic differential-pressure transmitters. These technologies can be used to improve existing DP level-measurement applications, and open up new areas where DP was not up to the task. ■

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Chemical Supply Chains Go Digital

When it comes to managing complex global supply chains, visibility and collaboration are the name of the game. To drive it, companies are embracing digital strategies

Keith Baranowski
SAP Ariba

The global chemical process industries (CPI) are undergoing a major transformation brought about by mergers, divestitures and shifting market dynamics, and these changes are leading to the creation of nonlinear supply chains. To keep pace, many industry leaders are harmonizing their supplier-management, sourcing and supply-chain processes using a digital strategy that enables them to extend business processes beyond the four walls of the enterprise. Along the way, these efforts are creating new efficiencies and cost savings that are helping them to compete in today's complex marketplace.

Industry trends prompt change

Shifting market dynamics. Across the CPI, competition is emerging from growth in the number of low-cost suppliers competing for business. These companies range from spinoffs of established providers, to firms in developing countries. Regardless of the source of the competition, an increasingly crowded field is leading to growing price and margin pressures. In addition, globalization and environmental trends are changing demand patterns. Customers require niche products to satisfy diverse local regulations and end users, while environmental concerns are changing how products are packaged.

For instance, consumers in many regions and many different industry segments prefer products with "green" packaging, often shifting demand away from plastics, shrinkwrap and other non-biodegradable packaging. This leads to further pressure on margins in these categories. And underlying commodity prices are unpredictable, making it difficult for operating companies to forecast and manage costs and profitability. Similarly, volatility in petroleum prices alone creates tremendous instability in an industry where petroleum and petroleum-derived raw materials and intermediates can represent more than one-tenth of the total spend.

Acquisitions, mergers and divestitures. As in many industries, chemical manufacturers are accelerating innovation in ways that create competitive advantage and grow corporate product portfolios. Market leaders are investing in innovation through internal R&D initiatives and their own venture capital arms. They are also adopting disruptive technologies and expanding their product portfolios by acquiring product lines from peers and competitors. These investments and acquisitions increase the urgency for — and the challenges of — harmonizing business processes and supply bases across disparate lines of business.

Business model and portfolio innovation and growth that depend on complex, global, nonlinear supply chains. To support these new business models and product portfolios, many CPI producers are taking advantage of trends such as toll manufacturing (when a third party performs a service related to a product for a volume-based fee, or toll, quickly and efficiently). Tolling can make costs more predictable because the toll manufacturer buys its own equipment and uses its own floor space — taking on huge costs (and risks) that the chemical manufacturer no longer needs to bear. In addition, toll manufacturing often helps companies become more agile at innovating, by allowing them to focus their resources and efforts on innovative opportunities, rather than on manufacturing.

Typically, companies see a 10% increase in new product revenue from accelerated innovation resulting from an extended ecosystem. But many also see a rise in risk, as dependency on global, nonlinear networks of toll manufacturers and other companies grows.

To manage this, CPI companies need deeper supply-chain visibility and improved collaboration with vendors. Visibility into the product quality of batches or lots produced by toll manufacturers, for instance, is critically important to ensure both customer satisfaction and regulatory compliance. Improved visibility into the availability of the supply also helps a company to ensure its ability to meet market demand.

The case for going digital

While the marketplace changes for chemical companies, advanced digital technologies such as connected devices, the Cloud, Big Data and the Internet of Things (IoT) are driving new opportunities to improve traditional value changes. In fact, IBM and IDC predict that total expected benefits from digital transformation is expected to amount to $14.4 trillion dollars by 2022.

Given these trends, it is more important than ever that chemical manufacturers transform from being essentially disconnected, manual organizations to becoming connected,

digital enterprises

1. Align digitization efforts with business imperatives. It is first important to define your digital vision, mapping out where you are and where you want to go. Decide what's most important for your company and ensure your digital strategy aligns with these goals. This includes determining the strategic relevance of different supply-chain planning functions, and identifying the value these elements may contribute to your competitive advantage.

2. Standardize and harmonize the process. To reduce complexity and streamline procurement processes across different lines of business and acquisitions, leading chemical manufacturers are transforming strategic procurement. Focusing on supplier qualification and selection processes, and harmonizing disparate supplier bases across different regions, can help you achieve purchasing scale in new ways that were previously not possible.

3. Collaborate with suppliers across plan-to-deliver processes. To harness global, nonlinear supply chains and achieve operational excellence, industry leaders are working to provide "a single face" to suppliers by eliminating fragmented communications. They are also collaborating with key direct trading partners, including toll manufacturers and suppliers in low-cost countries. These strategies can help to foster proactive supply chain visibility, increase flexibility and effectively manage volatility.

4. Ensure that your plans are agile and flexible. It may be beneficial to incrementally initiate these digital strategies across your enterprise. Benefits of agile deployment can include shorter time-to-market, early delivery of customer value, transparency and visibility, as well as early risk identification. This approach is not always easy to adopt, as it requires a flexible and ready-to-learn culture across the company. It may make sense to pick a specific area to start with and then scale up from there. If this is the strategy you choose to deploy, ensure that your strategy is flexible enough to move as you do.

Reaping the rewards

The benefits of digitization have been clearly and profoundly demonstrated in leading companies. McKinsey & Co. [1] has reported that business-to-business (B2B) companies that are digital leaders generate 8% higher shareholder returns, and a revenue compound annual growth rate (CAGR) that is five times greater, than their competitors. In addition, successful digitization can lead to:

- *Improved compliance through reduced risk in supplier selection and management.* By employing more sophisticated and granular supplier-qualification and management strategies, companies can enhance compliance on an ongoing basis, which helps to reduce financial, brand and other risks
- *Reduced costs by harmonizing processes*. Global companies that grow through acquisition and organic investment can gain the best of both worlds — benefiting from local and commodity ex-

CASE EXAMPLE: BASF'S DIGITAL TRANSFORMATION

BASF provides an example of the benefits that digitization can deliver. The global chemical company has essentially transformed its sourcing and supplier management across direct and indirect spend, ensuring that all goods and services that are both directly and indirectly incorporated into the products they are manufacturing are covered. In addition, BASF is packaging through the use of digital technologies such as business networks and cloud-based applications. The company started by deploying a new operating model that was structured around strategic category teams, shared-services procurement, and local procurement, to take advantage of local and commodity expertise and efficiencies. BASF then implemented digitized solutions to manage sourcing direct inputs into its products, such as raw materials. Efforts to qualify and segment suppliers by region, commodity and even at the local plant level, and to enforce qualification in its direct materials-sourcing processes, have yielded demonstrable returns. ■

pertise, and from the efficiencies that harmonized, shared-services organizations offer

- *Greater process efficiency.* Processes from sourcing and orders through invoice and payment run faster and smarter, because integration with enterprise resource planning (ERP) and supply-chain-optimization systems means connecting the people, partners, processes and information to effectively manage all source-to-settle activities
- *Increased inventory turns.* Supplier collaboration enables companies to reduce inventory levels, increase fill rates, and minimize supply chain risks through better supply chain visibility — all with minimal manual data entry and re-keying

Changing with the times

Digital transformation of value chains offers a massive opportunity for chemical companies to create new sustainable business and operational advantages. But success requires a change in mindset, and in many cases, will mean investment in new talent and technologies. The process will not be easy and success will not be realized overnight. But companies that commit to making the change will be rewarded in the end with more resilient and competitive supply chains that give them advantage, today and in the future. ■

Edited by Suzanne Shelley

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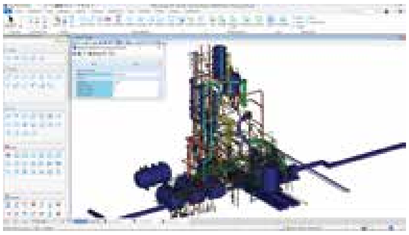
CONNECTEDPLANT CONFERENCE
Harnessing Digital Tools to Drive Success

The 2018 Connected Plant Conference (www.connectedplantconference.com) will take place February 26–28 in Charlotte, N.C. Focused on digitalization and connectivity trends in the chemical process industries (CPI), as well as the power-generation sector, the event's technical program boasts speakers from a wide range of companies, including experts from DuPont (Wilmington, Del.; www.dupont.com), Evonik Industries AG (Essen, Germany; www.evonik.com), The Dow Chemical Co. (Midland, Mich.; www.dow.com), Honeywell (Morris Plains, N.J.; www.honeywell.com) and more. These sessions intend to guide CPI professionals in the adoption and evolution of digital technologies, including data analytics, internet of things (IoT), smart sensing and monitoring devices, predictive diagnostics and more. The following is a selection of the technologies that will be highlighted at the Connected Plant Conference.



Bentley Systems

Collaboration leads to consistency with this design software

OpenPlant Connect Edition (photo) is a plant design software featuring a collaborative, 2- and 3-D design environment based on open data standards. The software supports cloud-based asset tag management and synchronization of lifecycle information with enterprise data stores. Increased collaborative capabilities improve consistency, as work can be easily coordinated and important deliverables can be shared within the extended supply chain, enforcing common standards across disciplines and organizations. Furthermore, the software supports faster multi-discipline design due to an updated interface and streamlined loading of data from other 3-D design applications. — *Bentley Systems, Inc., Exton, Pa.*
www.bentley.com

Mettler Toledo

This digital technology increases sensor uptime

Sensors equipped with Intelligent Sensor Management (ISM) technology (photo) are said to have longer service life and less unplanned downtime due to optimized maintenance scheduling and predictive diagnostics. Quicker installation and commissioning are possible thanks to self-configuring transmitters. Sensors feature high signal integrity, even over long cable runs and in humid conditions. ISM provides precise, realtime information on sensor health, helping to sustain measurement performance and avoid unplanned downtime. — *Mettler Toledo, Columbus, Ohio*
www.mt.com/pro

Seeq

Dynamic data visualization and reporting for process engineers

This company provides a visual analytics system for process data (photo) that enables engineers to rapidly investigate data stored in plant data historians without the need to duplicate databases. The Workbench application includes data visualization and modeling, as well as interactive tools for diagnostic, monitoring and predictive analytics. The Organizer application allows engineers to create documents that assemble analyses and visualizations into reports, presentations and meeting agendas. Documents created with Organizer are dynamic because they are directly tied to the underlying data and are time relative. — *Seeq, Seattle, Wash.*
www.seeq.com

Siemens

Create virtual-reality 3-D models using engineering data

The COMOS Walkinside platform (photo) enables the use of 3-D engineering data from the basic and detail engineering phases throughout the entire asset lifecycle. Highly complex process plants models can be represented realistically in three dimensions, with COMOS acting as a global data center. Up-to-date plant data are continuously available, and can be used not only for engineering and monitoring purposes, but also for operation and training, says the company. COMOS Walkinside offers solutions for building and viewing 3-D virtual-reality models. It can be used for immersive operator training and delivers tools for data exchange with third-party applications, as well as distributed realtime collaboration. — *Siemens AG, Munich, Germany*
www.siemens.com ■

Mary Page Bailey

Don't Forget the Advantages of Differential Pressure Flow Metering

In the world of process control, Differential Pressure (DP) flow measurement is often overlooked as a solid performer. This is especially true when looking into the measurement of hydrocarbon fluids in the chemical and petrochemical industries. The fact is that when combined with today's advanced pressure transmitter capabilities, DP technology outperforms many other flow measurement solutions.

Each of the higher-performing techniques available for DP flow measurement, including Venturi, Cone and Wedge meters, and Averaging Pitot Tubes, has its place in optimizing flow measurements in plant processes. All differential pressure flow meters can be employed for compensated mass flow with the addition of temperature and static pressure measurement. Most flow computers have compensation algorithms already in place that are based on the latest AGA and API standards, real gas laws, and other methods. Some multivariable transmitters have built-in flow equations, making them a combination transmitter/flow computer.

There are numerous attributes associated with DP meters: no moving parts, accuracies that rival turbine meters without the need for maintenance, temperature and pressure options galore, and service ranges from vacuum to many thousands of pounds per square inch.

Preso® Differential Pressure Cone Meter

The materials of construction for DP meters are very flexible. Most companies can manufacture out of whatever material best suits the application. Often times, it will be up to the end user to determine the materials most compatible with their processes.

If desired, most DP meter elements can be flow tested along with their respective transmitters for ultimate performance. Some meter designs can have transmitters directly mounted to the element with suitable manifolding to allow for future calibration checks and service.

Badger Meter offers a choice of advanced differential pressure flow meters. The company's Preso® line provides a custom engineered solution specifically manufactured to fit within the customer's system, ensuring a reliable long-term solution for a wide range of applications. Their fixed geometry will last for years, and when combined with advanced differential pressure transmitters, they deliver very good rangeability without the complexity that is common with old school analog transmitters. When used with a multivariable transmitter, Preso® DP meters are easily installed and durable in nature. This technology is a proven problem solver with versions that are specific to different measurement tasks.

www.badgermeter.com

BEUMER Group: Digital Transformation

Effectively shaping digital transformation

What will the world of logistics look like in a couple of years? Will drones with stock orders fly through storehouses, will robots deliver ordered goods to the final customer and will truck drivers activate 3D printers in their trailers to manufacture the order during transport?

Logistics is one of the industries where the influence of the digital transformation process is particularly strong. This is because digital logistics offers considerable potential when it comes to costs and speed. The smart integration of digital technologies can especially make intralogistics more efficient and environmentally safe.

PICTURE CREDITS: BEUMER GROUP GMBH & CO. KG

The new BEUMER app enables users to keep an eye on the current status of the machines connected to their system using their mobile devices

BEUMER Group takes an active part in shaping this change initiated by networking and digitalisation. In addition to know-how in terms of digital technologies and processes, a major challenge is to plan and realise digital innovation together with the customer. On the one hand, potential brought by digital innovation is to be anticipated in the existing product portfolio. On the other hand, the focus of digital transformation is set on new business segments opening up for BEUMER Group.

The customer is at the centre of all development of digital business models. Close and iterative coordination with and involvement of the customer is therefore a key prerequisite for digital transformation. For BEUMER Group's customers, this creates sustainable value for tomorrow's logistics.

BEUMER Group is an international leader in the manufacture of intralogistics systems for conveying, loading, palletising, packaging, sortation, and distribution. With 4,000 employees worldwide, BEUMER Group has annual sales of about EUR 750 million. The BEUMER Group and its group companies and sales agencies provide their customers with high-quality system solutions and an extensive customer support network around the globe and across a wide range of industries, including bulk materials and piece goods, food/non-food, construction, mail order, post, and airport baggage handling.

www.beumergroup.com

Condition Monitoring in the Cabinet

Turck's IMX12-CCM cabinet guard continuously monitors the relevant ambient data inside control cabinets and protective housings in hazardous and non-hazardous areas

As part of the diagnostic monitoring of devices in the field and control level, it is often the transmission routes and interfaces that are ignored. On-site cabinets with I/O systems – particularly in legacy installations – are thus nowadays often the Achilles heel of the installation technology. Condition monitoring here was previously only often possible with considerable effort. **Turck**'s IMX12-CCM cabinet guard offers an easy solution for reliable cabinet condition monitoring – also with existing installations. The device on the DIN rail monitors correct door closure, humidity and temperature, and outputs an alarm signal to the control level if the limit value is reached.

Turck's IM12-CCM (left) and the IMX12-CCM cabinet guards are designed for use in non-Ex and Ex areas

The new IMX12-CCM (Cabinet Condition Monitoring) cabinet guard indicates the degree of protection of the control cabinet with a single switch signal. The 12 mm wide device comes with an intrinsically safe 2-wire isolating transducer interface, enabling it to be used in explosion hazardous areas. This means that only a maximum of four wires and available space on a DIN rail are required to install and commission the IMX12-CCM. The teach-in process can be carried out without the need for a computer or an additional tool. The standard HART interface is provided for additional diagnostic options, such as for reading out the absolute measured values.

Besides the interface technology, Turck's control cabinet guard offers a range of sensors which monitor the actual status of the environment: a temperature sensor, an absolute humidity sensor and a triangulation sensor. In order to deal with instrumentation failure in advance, the IMX12-CCM monitors also long term trends and outputs a signal to the control level if limit values are exceeded. The cabinet guard continuously processes the recorded data of the sensors and compares it with the taught safe condition. This enables interventions to be made quickly and effectively.

www.turck.com/ccm

A choice of solutions for pressure regulation

Cashco has launched three new devices for the control of gas pressure

The new ULR-1 ("Un-Loading Regulator") valve from **Cashco** is more than an enhanced product. It also brings clarification and new information, says Clint Rogers, General Manager of Cashco's Valve Division.

The ULR-1 was originally marketed as the U1 by Kaye MacDonald, which Cashco bought in 1999. Unfortunately, the only documentation for the U1 and similar products was the original schematics, which showed how the tubing and fittings were to be installed, Rogers says.

"Previously, a customer would have had to locate the technical bulletin, work their way through its product coder and then a separate product coder for the correct bill of materials for the hookup," Rogers explains. "Not any more. With these new products, all of the information is in the technical bulletin and the operating manual."

As Rogers explains, the ULR-1 is a DA4 regulator with a Cashco CA1 back-pressure valve mounted onto it. Using the inlet pressure from the valve, the CA1 is set to control the outlet pressure of the main valve. Because the outlet of the CA1 constantly exhausts into the atmosphere, the media through the valve must be environmentally safe gas such as oxygen or nitrogen.

For even more choice in pressure regulation, Cashco has also introduced the SLR-1 and SLR-2 Self-Loading Regulators. The SLR-1 is a high-performance, pressure-loaded, pressure-reducing regulator with a self-contained regulator mounted onto it. Inlet pressure from the main valve is diverted to the pilot, which, in turn, reduces the loading pressure to the cover dome in order to maintain the set point of the main valve. The pressure inside the dome is static, so gas is only released to atmosphere when the outlet pressure setting is reduced or the system is shut down.

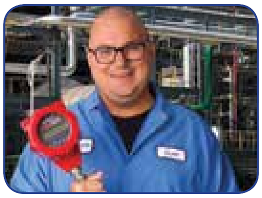
Cashco SLR-1 (left) and SLR-2 (right)

The new SLR-2 self-loading regulator is similar to the SLR-1, but its loading valve is not self-relieving. Instead, the cover dome bleeds through a filter and check valve back into the outlet of the main valve. This feature allows the SLR-2 to be marketed for hydrogen gas, natural gas and sour gas (NACE) applications.

www.cashco.com

Manage Your Flow Energy with ONE Complete Flow Energy Solution

Sierra offers turnkey solution for facilities managers & engineers to specify, commission, and maintain all gas, liquid, & steam flow meters with ONE company and proven flow expert



Sierra's Dedicated flow energy management expert for all gas, liquid, steam applications

Facilities managers and engineers at chemical plants have the challenging task of managing all the flow energy in their facility with the mandate from upper management to improve productivity and save money on energy costs. Flow energy is defined as "flows that cost money." These flows include natural gas, compressed air, water and steam. Many times different flow meter technologies are needed depending on the type of fluid being measured. In reality, a maintenance manager or engineer may be managing up to 20 different instrumentation companies for their gas, liquid, and steam measurements, an often time-consuming and frustrating process.

To simplify flow energy management, **Sierra** offers the Big-3 three revolutionary flow meter technologies all made by one USA company and supported globally by our network of over 150 locations in over 50 countries. The Big-3 includes: Sierra's QuadraTherm 640i/780i thermal mass flow meters ideal for gas flow measurement, the InnovaMass 240i/241i vortex flow meters for steam and the new InnovaSonic 207i ultrasonic flow meter for hot/chilled water.

Your dedicated Sierra flow experts will help you specify the right flow meters to answer key questions like: Why are your boilers running 24/7? How much money are you wasting on compressed air leaks? Why is your steam production so low? How much water are you using in your process? With Sierra as your flow energy management partner, you get one complete flow energy solution to make energy efficiency decisions clear and easy.

Perfect for plant automation, the Big-3 also share common firmware and software for easy integration, set up, and serviceability, enabling operators to leverage their knowledge between the different platforms. Big-3 software apps also give plant engineers and managers the ability to mine and analyze data quickly to make effective productivity decisions. All patented Big-3 (thermal, vortex, and ultrasonic) sensors provide unparalleled accuracy, extensive flow knowledge through multivariable functionality, and benefit from the Raptor operating system to manage sensor inputs.

The accuracy of the Big-3 is backed up with world-class calibration. Flow meters are only as good as their calibrations, and Sierra has invested millions in its state-of-the-art, fully automated, gas and liquid calibration facilities to assure consistent accuracy and repeatability of its flow meters. Sierra is ISO certified and follows ISO17025 guidelines. All Big-3 flow meters, come with a NIST traceable and fully ISO 17025 compliant Calibration Certification.

Sierra offers a FREE Flow Energy Review of your Plant, so you can save thousands in energy costs. To learn more, download at www.sierrainstruments.com/FlowEnergyGuide

www.sierrainstruments.com

Sensors join force to create new digital services

Endress+Hauser's cloud-based platform unveils hidden potential for business gains via the exchange of information between devices that are already installed on the plant

As a leading supplier of measuring instruments for industrial applications, **Endress+Hauser** sees great potential for new improvements in the further networking of assets. Endress+Hauser offers solutions to customers who can exploit this potential, and at the same time is positioning itself as a leading supplier in the Industrial Internet of Things (IIoT) market.

Collecting information on installed devices is the starting point for an IIoT strategy

An "Analytics" application – a web-based tool listing all the devices installed in the plant – is a simple and efficient way to bring order to asset management, especially since undocumented retrofits are not unusual in modern chemical plants. For Endress+Hauser devices, additional information displayed includes the current availability of the product and, if necessary, recommendations for substitutes. Based on the data collected, the tool can then present statistics on the installed base of devices and recommend ways to optimize it, with a view to simplifying plant operation and reducing costs.

The Analytics web application reads data by simply scanning the device nameplate with a smartphone app called Scanner App. Alternatively, Endress+Hauser's edge device – a smart gateway that is easy to set up – can be used with various bus systems; it automatically identifies each device and independently recognizes any changes.

Data security is important in a world where networking is rapidly spreading into all areas of life. On one hand, widespread data exchange between companies brings valuable benefits. On the other hand, it is essential to protect intellectual property. To ensure maximum data security, Endress+Hauser uses the most modern safety mechanisms, including:

- robust encryption with secure keys (HTTPS/TLS with SHA-256);
- data centers certified to European laws and standards such as ISO 27001; and
- an in-house platform with independent certification from EuroCloud.

Endress+Hauser is offering interested parties the chance to join the first market release and find out how to optimize their plant and processes.

Creating an installed base analysis of instrumentation, from whichever supplier, gives the plant operator an overview that helps to identify savings potentials, and enables a first step towards digitalizing the plant.

www.iiot.endress.com

Economic Indicators

2015 | 2016 | 2017

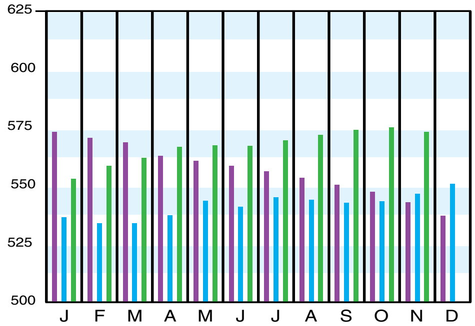
Download the CEPCI two weeks sooner at www.chemengonline.com/pci

CHEMICAL ENGINEERING PLANT COST INDEX (CEPCI)

(1957-59 = 100)	Nov. '17 Prelim.	Oct. '17 Final	Nov. '16 Final
CE Index	573.1	574.7	546.6
Equipment	692.5	694.4	654.1
Heat exchangers & tanks	604.5	610.0	567.6
Process machinery	692.5	690.6	663.5
Pipe, valves & fittings	900.1	900.3	818.9
Process instruments	411.7	409.0	394.0
Pumps & compressors	995.9	985.3	966.0
Electrical equipment	523.5	521.7	510.7
Structural supports & misc.	731.7	740.8	707.9
Construction labor	329.1	331.2	326.1
Buildings	567.4	565.6	546.0
Engineering & supervision	309.1	309.2	313.5

Starting with the April 2007 Final numbers, several of the data series for labor and compressors have been converted to accommodate series IDs that were discontinued by the U.S. Bureau of Labor Statistics

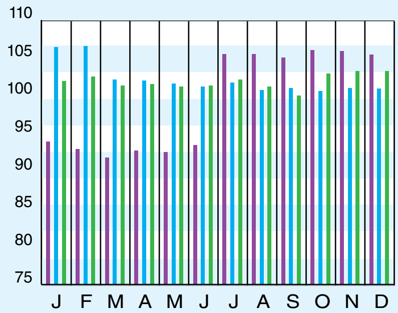
Annual Index:
2009 = 521.9
2010 = 550.8
2011 = 585.7
2012 = 584.6
2013 = 567.3
2014 = 576.1
2015 = 556.8
2016 = 541.7



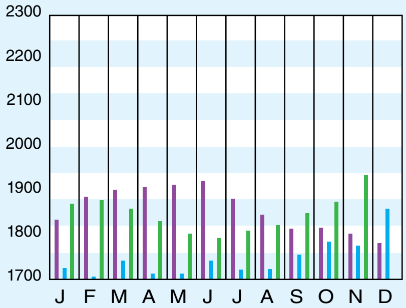
CURRENT BUSINESS INDICATORS

	LATEST	PREVIOUS		YEAR AGO
CPI output index (2012 = 100)	Dec. '17 = 103.2	Nov. '17 = 103.8	Oct. '17 = 102.8	Dec. '16 = 100.4
CPI value of output, $ billions	Nov. '17 = 1,937.0	Oct. '17 = 1,889.1	Sept. '17 = 1,856.7	Nov. '16 = 1,753.2
CPI operating rate, %	Dec. '17 = 77.1	Nov. '17 = 77.6	Oct. '17 = 76.8	Dec. '16 = 75.7
Producer prices, industrial chemicals (1982 = 100)	Dec. '17 = 269.8	Nov. '17 = 262.2	Oct. '17 = 262.5	Dec. '16 = 241.5
Industrial Production in Manufacturing (2012=100)*	Dec. '17 = 105.0	Nov. '17 = 104.9	Oct. '17 = 104.6	Dec. '16 = 102.6
Hourly earnings index, chemical & allied products (1992 = 100)	Dec. '17 = 181.5	Nov. '17 = 181.9	Oct. '17 = 182.5	Dec. '16 = 170.3
Productivity index, chemicals & allied products (1992 = 100)	Dec. '17 = 104.1	Nov. '17 = 103.5	Oct. '17 = 103.1	Dec. '16 = 103.5

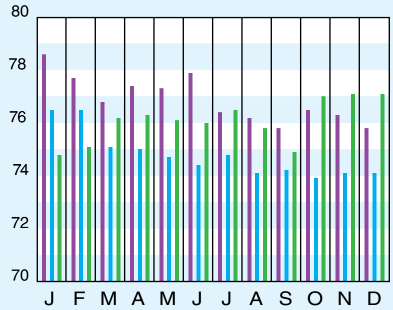
CPI OUTPUT INDEX (2000 = 100)†



CPI OUTPUT VALUE ($ BILLIONS)



CPI OPERATING RATE (%)



*Due to discontinuance, the Index of Industrial Activity has been replaced by the Industrial Production in Manufacturing index from the U.S. Federal Reserve Board.
†For the current month's CPI output index values, the base year was changed from 2000 to 2012
Current business indicators provided by Global Insight, Inc., Lexington, Mass.

CURRENT TRENDS

The preliminary value for the November *CE* Plant Cost Index (CEPCI; top; most recent available) decreased compared to the previous month's value, reversing an upward trend over the past four months. In addition, the final value for the October CEPCI was downwardly revised from the initial preliminary October value. Declines in the Equipment and Construction Labor subindices for November offset a small increase in the Buildings subindex to arrive at the lower CEPCI value for November. The Engineering & Supervision subindex fell by a small margin in November. The overall monthly CEPCI value for November 2017 stands at 4.8% higher than the corresponding value from November 2016.